V. M. Shabaev
Department of Physics, St. Petersburg State University,
Oulianovskaya Street 1, Petrodvorets, 198904 St. Petersburg,
Russia

The two-time Green function method in quantum electrodynamics of high-Z few-electron atoms is described in detail. This method provides a simple procedure for deriving formal expressions for the energy shift of a single level and for the energies and wave functions of degenerate and quasi-degenerate states. It also allows one to derive formal expressions for the transition and scattering amplitudes. Application of the method to resonance scattering processes yields a systematic theory for the spectral line shape. The practical ability of the method is demonstrated by deriving the formal expressions for the QED and interelectronic-interaction corrections to energy levels and transition and scattering amplitudes in one-, two-, and three-electron atoms. The resonance scattering of a photon by a one-electron atom is also considered.
PACS number(s): 12.20.-m, 12.20.Ds, 31.30. Jv

Contents

I. INTRODUCTION

A great progress in experimental investigations of high-Z few-electron systems (see, e.g., [1]) stimulated theorists to perform accurate QED calculations for these systems. The calculations of the QED and interelectronic-interaction corrections in high-Z few-electron systems are conveniently divided in two stages. The first stage consists in deriving formal expressions for these corrections from the first principles of QED. The second one consists in numerical evaluations of these expressions. The present paper will be completely focused on the first stage. As to the numerical evalutions of the QED corrections, they are recently reviewed in [2–6].

Historically, the first method suitable for derivation of the formal expressions for the energy shift of a bound state level was formulated by Gell-Mann, Low, and Sucher [7,8]. This method is based on introducing an adiabatically damped factor, $\exp(-\lambda|t|)$, in the interaction Hamiltonian and expressing the energy shift in terms of so-called adiabatic S_λ matrix elements. Due to its simple formulation, the Gell-Mann–Low–Sucher formula for the energy shift gained wide spreading in the literature related to high-Z few-electron systems [9–16]. However, the practical use of this method showed that it has several serious drawbacks. One of them consists in strong complication of the derivation of the formal expressions for so-called *reducible* diagrams. By the reducible diagrams we mean here the diagrams in which an intermediate state energy of the atom coincides with the reference state energy (this terminology is quite natural since it can be considered as an extension of the definitions introduced by Dyson [17] and by Bethe and Salpeter [18] to high-Z few-electron atoms). As to *irreducuble* diagrams, i.e. the diagrams in which the intermediate state energies differ from the reference state energy, the derivation of the formal expressions for them can easily be reduced to the usual ($\lambda = 0$) S-matrix elements in every method, including the Gell-Mann–Low–Sucher method as well (see, e.g., [11,15]), and, therefore, causes no problem. Another serious drawback of the Gell-Mann–Low–Sucher method consists in the fact that this method needs special studying the renormalization procedure since the adibatic S_λ-matrix is suffered from the ultraviolet divergences. Due to noncovariantness of the adiabatically damped factor, the ultraviolet divergences can not be removed from S_λ if $\lambda \neq 0$. However, from the physical point of view one may expect that these divergenes cancel each other in the expression for the energy shift and, therefore, may be disregarded in the calculation of the energy shift of a single level. But for the case of degenerate levels, this problem becomes very urgent since we can not expect that the standard renormalization procedure makes the secular operator to be finite in the ultraviolet limit [10,12]. In addition, we should note that at present there is no formalism based on the Gell-Mann–Low–Sucher approach which would provide treatment of quasidegenerate levels. To date, no formalism in the framework of this approach was developed for calculation of the transition or scattering amplitudes.

The same problems refer to the evolution operator method developed in [19–23].

Another way to formulate the perturbation theory for high-Z few-electron systems consists in using Green's functions. These functions contain the complete information about the energy levels and the transition and scattering amplitudes. The renormalization problem does not appear in this way since Green's functions can be renormalized from the very beginning (see, e.g., [24]). To date, various versions of the Green function formalism were developed which differ from each other by methods of extracting the physical information (the energy levels and the transition and scattering amplitudes) from Green's functions. One of these methods was worked out in [25–29] and was successfully employed in many practical calculations [30–41]. Since one of the key elements of this methods consists in using two-time Green's functions, in what follows we will call it as the two-time Green function (TTGF) method. This method, which provided solving all the problems appeared in the other formalisms indicated above, will be considered in detail in the present paper.

As to other versions of the Green function method [12,43–51,16], a detailed discussion of them would be beyond the scope of the present paper. We note only that some of these methods are also based on employing two-time Green function's but yield other forms of the perturbation theory. So, in [12,44–47] the two-time Green functions were used for constructing quasipotential equations for high-Z few-electron systems. It corresponds to the perturbation theory in the Brillouin-Wigner form while the method of Refs. [25–29] yields the perturbation theory in the Rayleigh-Schrödinger form. Various versions of the Bethe-Salpeter equation derived from the $2N$-time Green function formalism for high-Z few-electron systems can be found in [12,48]. In [49,50] the perturbation theory in the Rayleigh-Schrödinger form is constructed in the case of a one-electron system where the problem of relative electron times is absent.

The relativistic unit system ($\hbar = c = 1$) and the Heaviside charge unit ($\alpha = \frac{e^2}{4\pi}, e < 0$) are used in the paper.

II. ENERGY LEVELS OF ATOMIC SYSTEMS

In this section we formulate the perturbation theory for calculation of the energy levels in high-Z few-electron atoms. In these systems the number of the electrons, which we denote by N, is much smaller than the nuclear charge number Z. It follows that the interaction of the electrons with each other and with the quantized electromagnetic

field is much smaller (by factors $1/Z$ and α, respectively) than the interaction of the electrons with the Coulomb field of the nucleus. Therefore, it is natural to assume that in zeroth approximation the electrons interact only with the Coulomb field of the nucleus and obey the Dirac equation

$$(-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta m+V_{\rm C}(\mathbf{x}))\psi_n(\mathbf{x})=\varepsilon_n\psi_n(\mathbf{x})\,. \tag{2.1}$$

The interaction of the electrons with each other and with the quantized electromagnetic field is accounted by perturbation theory. In this way we get the quantum electrodynamics in the Furry picture. It should be noted that we could start also with the Dirac equation with an effective potential $V_{\rm eff}(\mathbf{x})$ which describes approximately the interaction with the other electrons. In this case the interaction with the potential $\delta V(\mathbf{x})=V_{\rm C}(\mathbf{x})-V_{\rm eff}(\mathbf{x})$ must be accounted for perturbatively. Using the effective potential provides an extention of the theory to many-electron atoms where, for instance, a local version of the Hartree-Fock potential can be used as $V_{\rm eff}(\mathbf{x})$. However, for simplicity, in what follows we will assume that in zeroth approximation the electrons interact only with the Coulomb field of the nucleus.

In the present paper we will mainly consider the perturbation theory with the standard QED vacuum. The transition to the formalism in which the role of the vacuum is played by closed shells is realized by replacing $i0$ with $-i0$ in the electron propagator denominators corresponding to the closed shells.

Before to formulate the perturbation theory for calculations of the interelectronic interaction and radiative corrections to the energy levels, we consider standard equations of the Green function approach in quantum electrodynamics.

A. $2N$-time Green function

It can be shown that the complete information about the energy levels of an N-electron atom is contained in Green's function defined as

$$G(x_1',\dots x_N';x_1,\dots x_N)=\langle 0|T\psi(x_1')\cdots\psi(x_N')\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle\,, \tag{2.2}$$

where $\psi(x)$ is the electron-positron field operator in the Heisenberg representation, $\overline{\psi}(x)=\psi^\dagger\gamma^0$, and T is the time-ordered product operator. The basic equations of the quantum electrodynamics in the Heisenberg representation are summarized in Appendix A. The equation (2.2) presents a standard definition of $2N$-time Green's function which is a fundamental object of the quantum electrodynamics. It can be shown (see, e.g., [24,52]) that in the interaction representation the Green function is given by

$$\begin{aligned}
&G(x_1',\dots x_N';x_1,\dots x_N)\\
&=\frac{\langle 0|T\psi_{\rm in}(x_1')\cdots\psi_{\rm in}(x_N')\overline{\psi}_{\rm in}(x_N)\cdots\overline{\psi}_{\rm in}(x_1)\exp\{-i\int d^4z\mathcal{H}_I(z)\}|0\rangle}{\langle 0|T\exp\{-i\int d^4z\mathcal{H}_I(z)\}|0\rangle} \qquad (2.3)\\
&=\Big\{\sum_{m=0}^{\infty}\frac{(-i)^m}{m!}\int d^4y_1\cdots d^4y_m\langle 0|T\psi_{\rm in}(x_1')\cdots\psi_{\rm in}(x_N')\overline{\psi}_{\rm in}(x_N)\cdots\overline{\psi}_{\rm in}(x_1)\\
&\quad\times\mathcal{H}_I(y_1)\cdots\mathcal{H}_I(y_m)|0\rangle\Big\}\Big\{\sum_{l=0}^{\infty}\frac{(-i)^l}{l!}\int d^4z_1\cdots d^4z_l\langle 0|\mathcal{H}_I(z_1)\cdots\mathcal{H}_I(z_l)|0\rangle\Big\}^{-1} \qquad (2.4)
\end{aligned}$$

where

$$\mathcal{H}_I(x)=\frac{e}{2}\,[\overline{\psi}_{\rm in}(x)\gamma_\mu,\psi_{\rm in}(x)]A^\mu_{in}(x)-\frac{\delta m}{2}\,[\overline{\psi}_{\rm in}(x),\psi_{\rm in}(x)] \tag{2.5}$$

is the interaction Hamiltonian. Commutators in equation (2.5) refer to operators only. The first term in (2.5) describes the interaction of the electron-positron field with the quantized electromagnetic field and the second one is the mass renormalization counterterm. We consider here that the interaction of the electrons with the Coulomb field of the nucleus is included into the unperturbed Hamiltonian (the Furry picture). However, there is also an alternative method to get the Furry picture. In this method the interaction with the Coulomb field of the nucleus is included in the interaction Hamiltonion and the Furry picture is obtained by summing infinite sequences of Feynman diagrams describing the interaction of electrons with the Coulomb potential. As a result of this summation, the free-electron propagators are replaced by the bound-electron propagators. This method is very convenient for studying processes involving continuum-electron states and will be used in the section concerning the radiative recombination process.

The Green function G is constructed by perturbation theory according to equation (2.4). This is carried out with the aid of Wick's theorem (see, e.g., [24]). According to this theorem the time-ordered product of field operators is equal to the sum of normal-ordered products with all possible contractions between the operators

$$T(ABCD\cdots) = N(ABCD\cdots) + N(A^aB^aCD\cdots) + N(A^aBC^aD\cdots) + \text{all possible contractions}\,, \tag{2.6}$$

where N is the normal-ordered product operator and the superscripts denote the contraction between the corresponding operators. The contraction between neighbouring operators is defined by

$$A^aB^a = T(AB) - N(AB) = \langle 0|T(AB)|0\rangle\,. \tag{2.7}$$

If the contracted operators are boson's operators they can be put one next to another. If the contracted operators are fermion's operators they also can be put one next to another but in this case the expression must be multiplied with the parity of the permutation of fermionic operators. Since in the Green function the vacuum expectation value is calculated, only the term with all contracted operators survives on the right-hand side of equation (2.6). In contrast to the free-electron QED, in the Furry picture the time-ordered product of two fermions operators must be defined also for the equal-time case to produce the correct vacuum polarization terms. As was noticed in [53], the definition

$$T[A(t)B(t)] = \frac{1}{2}A(t)B(t) - \frac{1}{2}B(t)A(t) \tag{2.8}$$

provides the following simple rule for dealing with the interaction operator. It can be written as

$$\mathcal{H}_I(x) = e\,\overline{\psi}_{\rm in}(x)\gamma_\mu\psi_{\rm in}(x)A^\mu_{in}(x) - \delta m\,\overline{\psi}_{\rm in}(x)\psi_{\rm in}(x) \tag{2.9}$$

and then Wick's theorem is applied with contractions between all operators, including equal-time operators. We note that the problem of the definition of the time-ordered product of fermion operators at equal times does not appear at all if the alternative method for producing the Furry picture discussed above is employed.

The contractions between the electron-positron fields and between the photon fields lead to the following propagators

$$\langle 0|T\psi_{\rm in}(x)\overline{\psi}_{\rm in}(y)|0\rangle = \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{\psi_n(\mathbf{x})\overline{\psi}_n(\mathbf{y})}{\omega - \varepsilon_n(1-i0)}\exp\left[-i\omega(x^0-y^0)\right] \tag{2.10}$$

and

$$\langle 0|TA^\mu_{\rm in}(x)A^\nu_{\rm in}(y)|0\rangle = -ig^{\mu\nu}\int\frac{d^4k}{(2\pi)^4}\frac{\exp\left[-ik\cdot(x-y)\right]}{k^2+i0}\,. \tag{2.11}$$

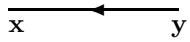
Here the Feynman gauge is considered. In equation (2.10) the label n runs over all bound and continuum states.

The denominator in equation (2.3) describes unobservable vacuum-vacuum transitions and, as one can show (see, e.g., [24]), it cancels disconnected vacuum-vacuum subdiagrams from the nominator. Therefore, we can simply omit all diagrams containing disconnected vacuum-vacuum subdiagrams in the nominator and replace the denominator by 1.

In practical calculations of the Green function it is convenient to work with the Fourier transform with respect to time variables

$$\begin{aligned} &G((p'^0_1,\mathbf{x}'_1),\ldots,(p'^0_N,\mathbf{x}'_N);(p^0_1,\mathbf{x}_1),\ldots,(p^0_N,\mathbf{x}_N)) \\ &= (2\pi)^{-2N}\int_{-\infty}^{\infty} dx^0_1\cdots dx^0_N dx'^0_1\cdots dx'^0_N \\ &\quad\times\exp\left(ip'^0_1x'^0_1+\cdots+ip'^0_Nx'^0_N - ip^0_1x^0_1-\cdots-ip^0_Nx^0_N\right) \\ &\quad\times G(x'_1,...,x'_N;x_1,...,x_N)\,. \end{aligned} \tag{2.12}$$

For the Green function $G((p'^0_1,\mathbf{x}'_1),\ldots,(p'^0_N,\mathbf{x}'_N);(p^0_1,\mathbf{x}_1),\ldots,(p^0_N,\mathbf{x}_N))$ the following Feynman rules can be derived:
(1) External electron line

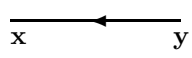


$\frac{i}{2\pi}S(\omega,\mathbf{x},\mathbf{y})\,,$

where

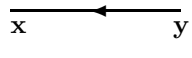
$$S(\omega,\mathbf{x},\mathbf{y}) = \sum_n \frac{\psi_n(\mathbf{x})\overline{\psi}_n(\mathbf{y})}{\omega-\varepsilon_n(1-i0)}\,, \tag{2.13}$$

$\psi_n(\mathbf{x})$ are solutions of the Dirac equation (2.1).
(2) Internal electron line



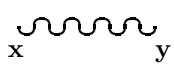
$\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\ S(\omega,\mathbf{x},\mathbf{y})\,.$

(3) Disconnected electron line



$\frac{i}{2\pi}S(\omega,\mathbf{x},\mathbf{y})\delta(\omega-\omega')\,.$

(4) Internal photon line



$\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega D_{\rho\sigma}(\omega,\mathbf{x}-\mathbf{y})\,,$

where, for zero photon mass, $D_{\rho\sigma}(\omega,\mathbf{x}-\mathbf{y})$ is given by

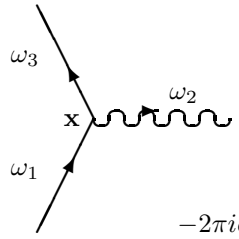
$$D_{\rho\sigma}(\omega,\mathbf{x}-\mathbf{y}) = -g_{\rho\sigma}\int \frac{d\mathbf{k}}{(2\pi)^3}\,\frac{\exp\left(i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right)}{\omega^2-\mathbf{k}^2+i0} \tag{2.14}$$

in the Feynman gauge and by

$$D_{00}(\omega,\mathbf{x}-\mathbf{y}) = \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\ ,\quad D_{i0}=D_{0i}=0 \qquad (i=1,2,3)\,, \tag{2.15}$$

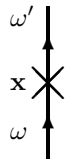
$$D_{il}(\omega,\mathbf{x}-\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\exp\left(i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right)}{\omega^2-\mathbf{k}^2+i0}\Big(\delta_{il}-\frac{k_ik_l}{\mathbf{k}^2}\Big) \qquad (i,l=1,2,3)\,, \tag{2.16}$$

in the Coulomb gauge.
(5) Vertex



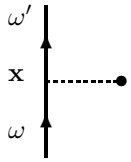
$-2\pi i e\gamma^\rho\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{x}\,.$

(6) The mass counterterm



$2\pi i\delta(\omega-\omega')\delta m\int d\mathbf{x}\,.$

(7) Symmetry factor $(-1)^P$, where P is the parity of the permutation of the final electron coordinates with respect to the initial ones.
(8) For every closed electron loop a minus sign is added.
(9) If, in addition, an external potential $\delta V(\mathbf{x})$ is present, an additional vertex appears



$$-2\pi i\gamma^0\delta(\omega-\omega')\int d\mathbf{x}\,\delta V(\mathbf{x})\,.$$

In principle, the Green function G contains the complete information about the energy levels of the atomic system. This can be shown by deriving the spectral representation for G. However, it is a hard task to extract this information directly from G since it depends on $2(N-1)$ relative times (energies) in the time (energy) representation. As we will see in the next section, the two-time Green function defined as

$$\widetilde{G}(t',t)\equiv G(t'_1=t'_2=\cdots t'_N\equiv t';t_1=t_2=\cdots t_N\equiv t) \tag{2.17}$$

also contains the complete information about the energy levels, and it is a much simpler task to extract the energy levels from $\widetilde{G}$.

B. Two-time Green function and its analytical properties

Let us introduce the Fourier transform of the two-time Green function by

$$\begin{aligned}\mathcal{G}(E;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_N)\delta(E-E') &= \frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty}dx^0dx'^0\exp\left(iE'x'^0-iEx^0\right)\\ &\times\langle 0|T\psi(x'^0,\mathbf{x}'_1)\cdots\psi(x'^0,\mathbf{x}'_N)\overline{\psi}(x^0,\mathbf{x}_N)\cdots\overline{\psi}(x^0,\mathbf{x}_1)|0\rangle\,,\end{aligned} \tag{2.18}$$

where, as in (2.2), the Heisenberg representation for the electron-positron field operators is used. Defined by equation (2.18) for real E, the Green function $\mathcal{G}$ can be continued analytically to the complex E plane. Analytical properties of this type Green functions in the complex E plane were studied in various fields of physics (see, e.g., [54–56]). In quantum field theory they were considered in detail by Logunov and Tavkhelidze in Ref. [57] (see also Ref. [58]), where the two-time Green function was employed for constructing a quasipotential equation. To study the analytical properties of the two-time Green function we derive the spectral representation for $\mathcal{G}$. Using the time-shift transformation rule for the Heisenberg operators (see Appendix A)

$$\psi(x^0,\mathbf{x})=\exp\left(iHx^0\right)\psi(0,\mathbf{x})\exp\left(-iHx^0\right) \tag{2.19}$$

and the equations

$$H|n\rangle=E_n|n\rangle\,,\qquad\qquad\sum_n|n\rangle\langle n|=I\,, \tag{2.20}$$

where H is the Hamiltonian of the system in the Heisenberg representation, we find

$$\begin{aligned}&\mathcal{G}(E;\mathbf{x}'_1,...,\mathbf{x}'_N;\mathbf{x}_1,...,\mathbf{x}_N)\delta(E-E')\\ &=\frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty}dx^0dx'^0\,\exp\left(iE'x'^0-iEx^0\right)\\ &\times\Big\{\theta(x'^0-x^0)\sum_n\exp\left[i(E_0-E_n)(x'^0-x^0)\right]\langle 0|\psi(0,\mathbf{x}'_1)\cdots\psi(0,\mathbf{x}'_N)|n\rangle\\ &\times\langle n|\overline{\psi}(0,\mathbf{x}_N)\cdots\overline{\psi}(0,\mathbf{x}_1)|0\rangle+(-1)^{N^2}\theta(x^0-x'^0)\sum_n\exp\left[i(E_0-E_n)(x^0-x'^0)\right]\\ &\times\langle 0|\overline{\psi}(0,\mathbf{x}_N)\cdots\overline{\psi}(0,\mathbf{x}_1)|n\rangle\langle n|\psi(0,\mathbf{x}'_1)\cdots\psi(0,\mathbf{x}'_N)|0\rangle\Big\}\,.\end{aligned} \tag{2.21}$$

Denoting, for simplicity, $E_n\equiv E_n-E_0$ (it corresponds to choosing the vacuum energy as the origin of reference) and taking into account that

$$\int_{-\infty}^{\infty} dx^0 dx'^0\, \theta(x'^0 - x^0) \exp\left[-iE_n(x'^0 - x^0)\right] \exp\left[i(E'x'^0 - Ex^0)\right]$$
$$= 2\pi\delta(E' - E)\frac{i}{E - E_n + i0}\,, \tag{2.22}$$
$$\int_{-\infty}^{\infty} dx^0 dx'^0\, \theta(x^0 - x'^0) \exp\left[-iE_n(x^0 - x'^0)\right] \exp\left[i(E'x'^0 - Ex^0)\right]$$
$$= -2\pi\delta(E' - E)\frac{i}{E + E_n - i0}\,, \tag{2.23}$$

we obtain

$$\mathcal{G}(E) = \sum_n \frac{\Phi_n \overline{\Phi}_n}{E - E_n + i0} - (-1)^N \sum_n \frac{\Xi_n \overline{\Xi}_n}{E + E_n - i0}\,, \tag{2.24}$$

where the variables $\mathbf{x}'_1, ..., \mathbf{x}'_N, \mathbf{x}_1, ..., \mathbf{x}_N$ are implicit and

$$\Phi_n(\mathbf{x}_1, ...\mathbf{x}_N) = \frac{1}{\sqrt{N!}}\langle 0|\psi(0, \mathbf{x}_1)\cdots\psi(0, \mathbf{x}_N)|n\rangle\,, \tag{2.25}$$
$$\Xi_n(\mathbf{x}_1, ...\mathbf{x}_N) = \frac{1}{\sqrt{N!}}\langle n|\psi(0, \mathbf{x}_1)\cdots\psi(0, \mathbf{x}_N)|0\rangle\,. \tag{2.26}$$

In equation (2.24) the summation runs over all bound and continuum states of the system of the interacting fields. Let us introduce the functions

$$A(E; \mathbf{x}'_1, ..., \mathbf{x}'_N; \mathbf{x}_1, ..., \mathbf{x}_N) = \sum_n \delta(E - E_n)\Phi_n(\mathbf{x}'_1, ..., \mathbf{x}'_N)\overline{\Phi}_n(\mathbf{x}_1, ..., \mathbf{x}_N)\,, \tag{2.27}$$
$$B(E; \mathbf{x}'_1, ..., \mathbf{x}'_N; \mathbf{x}_1, ..., \mathbf{x}_N) = \sum_n \delta(E - E_n)\Xi_n(\mathbf{x}'_1, ..., \mathbf{x}'_N)\overline{\Xi}_n(\mathbf{x}_1, ..., \mathbf{x}_N)\,. \tag{2.28}$$

These functions satisfy the conditions

$$\int_{-\infty}^{\infty} dE A(E; \mathbf{x}'_1, ..., \mathbf{x}'_N; \mathbf{x}_1, ..., \mathbf{x}_N) = \frac{1}{N!}\langle 0|\psi(0, \mathbf{x}'_1)\cdots\psi(0, \mathbf{x}'_N)$$
$$\times\overline{\psi}(0, \mathbf{x}_N)\cdots\overline{\psi}(0, \mathbf{x}_1)|0\rangle\,, \tag{2.29}$$
$$\int_{-\infty}^{\infty} dE B(E; \mathbf{x}'_1, ..., \mathbf{x}'_N; \mathbf{x}_1, ..., \mathbf{x}_N) = \frac{1}{N!}\langle 0|\overline{\psi}(0, \mathbf{x}_N)\cdots\overline{\psi}(0, \mathbf{x}_1)$$
$$\times\psi(0, \mathbf{x}'_1)\cdots\psi(0, \mathbf{x}'_N)|0\rangle\,. \tag{2.30}$$

In terms of these functions, the equation (2.24) is

$$\mathcal{G}(E) = \int_0^{\infty} dE' \frac{A(E')}{E - E' + i0} - (-1)^N \int_0^{\infty} dE' \frac{B(E')}{E + E' - i0}\,, \tag{2.31}$$

where we have omitted the varables $\mathbf{x}_1, ..., \mathbf{x}_N, \mathbf{x}'_1, ..., \mathbf{x}'_N$ and have taken into account that $A(E') = B(E') = 0$ for $E' < 0$ since $E_n \geq 0$. In fact, due to the charge conservation, only states with electric charge eN contribute to A in the sum over n in the right-hand side of equation (2.27) and only states with electric charge $-eN$ contribute to B in the sum over n in the right-hand side of equation (2.28). This can easily be shown by using the following commutation relations

$$[Q, \psi(x)] = -e\psi(x)\,, \qquad [Q, \overline{\psi}(x)] = e\overline{\psi}(x)\,, \tag{2.32}$$

where Q is the charge operator in the Heisenberg representation. Therefore, the equation (2.31) can be written as

$$\mathcal{G}(E) = \int_{E^{(+)}_{\min}}^{\infty} dE' \frac{A(E')}{E - E' + i0} - (-1)^N \int_{E^{(-)}_{\min}}^{\infty} dE' \frac{B(E')}{E + E' - i0}\,, \tag{2.33}$$

where $E^{(+)}_{\min}$ is the minimal energy of states with electric charge eN and $E^{(-)}_{\min}$ is the minimal energy of states with electric charge $-eN$. So far we considered $\mathcal{G}(E)$ for real E. The equation (2.33) shows that the Green function $\mathcal{G}(E)$

is the sum of Cauchy's type integrals. Using the fact that the integrals $\int_{E_{\rm min}^{(+)}}^{\infty} dE A(E)$ and $\int_{E_{\rm min}^{(-)}}^{\infty} dE B(E)$ converge (see equations (2.29), (2.30)), with the help of standard mathematical methods, one can show that the equation

$$\mathcal{G}(E) = \int_{E_{\rm min}^{(+)}}^{\infty} dE' \frac{A(E')}{E - E'} - (-1)^N \int_{E_{\rm min}^{(-)}}^{\infty} dE' \frac{B(E')}{E + E'} \tag{2.34}$$

defines an analytical function of E in the complex E plane with the cuts $(-\infty, E_{\rm min}^{(-)}]$ and $[E_{\rm min}^{(+)}, \infty)$ (see Fig. 1). This equation provides the analytical continuation of the Green function to the complex E plane. According to (2.33), to get the Green function for real E we have to approach the right-hand cut from the upper half-plane and the left-hand cut from the lower half-plane.

In what follows we will be interested in bound states of the system. According to equations (2.24)-(2.34) the bound states correspond to the poles of the function $\mathcal{G}(E)$ on the right-hand real semiaxis. In the zeroth approximation, when the interaction between the electron-positron field and the electromagnetic field is switched off, the poles corresponding to bound states are isolated (see Fig. 2). Switching on the interaction between the fields transforms the isolated poles into the branch points. It is caused by the fact that due to zero photon mass the bound states are no longer isolated points of the spectrum. Disregarding the instability of excited states, the singularities of the Green function $\mathcal{G}(E)$ are shown in Fig. 3. The poles corresponding to the bound states lie on the upper boundary of the cut starting from the pole corresponding to the ground state. It is natural to assume that $\mathcal{G}(E)$ can be continued analytically under the cut, to the second sheet of the Riemann surface. As a result of this continuation the singularities of $\mathcal{G}(E)$ can be turned down as displayed in Fig. 4.

In fact due to instability of excited states the energies of these states have small imaginary components and, therefore, the related poles lie slightly below the right-hand real semiaxis (Fig. 5). However, in calculations of the energy levels and the transition and scattering amplitudes of non-resonance processes we will neglect the instability of the excited states and, therefore, will assume that the poles lie on the real axis. The imaginary parts of the energies will be taken into account when we will consider the resonance scattering processes.

To formulate the perturbation theory for calculatons of the energy levels and the transition and scattering amplitudes we will need to isolate the poles corresponding to the bound states from the related cuts. It can be done by introducing a non-zero photon mass μ which is generally assumed to be larger than the energy shift (or the energy splitting) of the level (levels) under consideration and much smaller than the distance to other levels. The singularities of $\mathcal{G}(E)$ with non-zero photon mass, including one- and two-photon spectra, are shown in Fig. 6. As one can see from this figure, introducing the photon mass makes the poles corresponding to the bound states to be isolated.

In every finite order of the perturbation theory the singularities of the Green function $\mathcal{G}(E)$ in the complex E-plane are defined by the unperturbed Hamiltonian. In quantum mechanics this fact easily follows from the expansion of the Green function $(E - H)^{-1} = (E - H_0 - \delta V)^{-1}$ in powers of the perturbation potential δV

$$(E - H)^{-1} = \sum_{n=0}^{\infty} (E - H_0)^{-1} [\delta V (E - H_0)^{-1}]^n \,. \tag{2.35}$$

As one can see from this equation, in n-th order of the perturbation theory the Green function has poles of all orders till $n + 1$ at the unperturbed positions of the bound state energies. This fact remains also valid in quantum electrodynamics for $\mathcal{G}(E)$ defined above. It can easily be checked for every specific diagram in first and second orders in α. A general proof for an arbitrary diagram is given in Appendix B.

C. Energy shift of a single level

Let we are interested in the energy shift $\Delta E_a = E_a - E_a^{(0)}$ of a single isolated level a of an N-electron atom due to the interaction. The unperturbed energy $E_a^{(0)}$ is equal to the sum of the one-electron Dirac-Coulomb energies

$$E_a^{(0)} = \varepsilon_{a_1} + \cdots + \varepsilon_{a_N} \,, \tag{2.36}$$

which are defined by the Dirac equation (2.1). In a simple case the unperturbed wave function $u_a(\mathbf{x}_1, ..., \mathbf{x}_N)$ is a one-determinant function

$$u_a(\mathbf{x}_1, ..., \mathbf{x}_N) = \frac{1}{N!} \sum_P (-1)^P \psi_{Pa_1}(\mathbf{x}_1) \cdots \psi_{Pa_n}(\mathbf{x}_N) \,, \tag{2.37}$$

where ψ_n are the one-electron Dirac wave functions defined by equation (2.1) and P is the permutation operator. In a general case the unperturbed wave function is a linear combination of the one-determinant functions

$$u_a(\mathbf{x}_1, ..., \mathbf{x}_N) = \sum_b C_a^b \frac{1}{N!} \sum_P (-1)^P \psi_{Pb_1}(\mathbf{x}_1) \cdots \psi_{Pb_n}(\mathbf{x}_N) \,. \tag{2.38}$$

Let us introduce the Green function $g_{aa}(E)$ by

$$\begin{aligned} g_{aa}(E) &= \langle u_a | \mathcal{G}(E) \gamma_1^0 \cdots \gamma_N^0 | u_a \rangle \\ &\equiv \int d\mathbf{x}_1 \cdots d\mathbf{x}_N d\mathbf{x}'_1 \cdots d\mathbf{x}'_N u_a^\dagger(\mathbf{x}'_1, ..., \mathbf{x}'_N) \\ &\quad \times \mathcal{G}(E, \mathbf{x}'_1, ..., \mathbf{x}'_N; \mathbf{x}_1, ..., \mathbf{x}_N) \gamma_1^0 \cdots \gamma_N^0 u_a(\mathbf{x}_1, ..., \mathbf{x}_N) \,. \end{aligned} \tag{2.39}$$

From the spectral representation for $\mathcal{G}(E)$ (see equations (2.24)-(2.34)) we have

$$g_{aa}(E) = \frac{A_a}{E - E_a} + \text{terms that are regular at } E \sim E_a \,, \tag{2.40}$$

where

$$\begin{aligned} A_a = \frac{1}{N!} \int d\mathbf{x}_1 \cdots d\mathbf{x}_N d\mathbf{x}'_1 \cdots d\mathbf{x}'_N \, u_a^\dagger(\mathbf{x}'_1, \ldots, \mathbf{x}'_N) \langle 0 | \psi(0, \mathbf{x}'_1) \cdots \psi(0, \mathbf{x}'_N) | a \rangle \\ \times \langle a | \psi^\dagger(0, \mathbf{x}_N) \cdots \psi^\dagger(0, \mathbf{x}_1) | 0 \rangle u_a(\mathbf{x}_1, \ldots, \mathbf{x}_N) \end{aligned} \tag{2.41}$$

We assume here that a non-zero photon mass μ is introduced to isolate the pole corresponding to the bound state a from the related cut. We consider that the photon mass is larger than the energy shift under consideration and much smaller than the distance to other levels. To generate the perturbation series for E_a it is convenient to use a contour integral formalism developed first in the operator theory by Szökefalvi-Nagy and Kato [59–64]. Choosing a contour Γ in the complex E plane so that it surrounds the pole corresponding to the level a and keeps outside all other singularities (see Fig. 7) we have

$$\frac{1}{2\pi i} \oint_\Gamma dE E g_{aa}(E) = E_a A_a \,, \tag{2.42}$$

$$\frac{1}{2\pi i} \oint_\Gamma dE g_{aa}(E) = A_a \,. \tag{2.43}$$

Here we have assumed that the contour Γ is oriented anticlockwise. Dividing the equation (2.42) by (2.43) we obtain

$$E_a = \frac{\frac{1}{2\pi i} \oint_\Gamma dE E g_{aa}(E)}{\frac{1}{2\pi i} \oint_\Gamma dE g_{aa}(E)} \tag{2.44}$$

It is convenient to transform the equation (2.44) to the form that directly yields the energy shift $\Delta E_a = E_a - E_a^{(0)}$. In zeroth order, substituting into equations (2.25) and (2.26) the operators

$$\psi_{\text{in}}(0, \mathbf{x}) = \sum_{\varepsilon_n > 0} b_n \psi_n(\mathbf{x}) + \sum_{\varepsilon_n < 0} d_n^\dagger \psi_n(\mathbf{x}) \,, \tag{2.45}$$

$$\overline{\psi}_{\text{in}}(0, \mathbf{x}) = \sum_{\varepsilon_n > 0} b_n^\dagger \overline{\psi}_n(\mathbf{x}) + \sum_{\varepsilon_n < 0} d_n \overline{\psi}_n(\mathbf{x}) \tag{2.46}$$

instead of $\psi(0, \mathbf{x})$ and $\overline{\psi}(0, \mathbf{x})$, respectively, and considering the states $|n\rangle$ in (2.25) and (2.26) as unperturbed states in Fock's space, from equations (2.24)-(2.26), (2.39) one finds

$$g_{aa}^{(0)} = \frac{1}{E - E_a^{(0)}} \,. \tag{2.47}$$

This equation can also be derived using the Feynman rules for G (see below). Denoting $\Delta g_{aa} = g_{aa} - g_{aa}^{(0)}$, from (2.44) we obtain the desirable formula [25]

$$\Delta E_a = \frac{\frac{1}{2\pi i}\oint_\Gamma dE(E - E_a^{(0)})\Delta g_{aa}(E)}{1 + \frac{1}{2\pi i}\oint_\Gamma dE \Delta g_{aa}(E)}\,. \tag{2.48}$$

The Green function $\Delta g_{aa}(E)$ is constructed by perturbation theory

$$\Delta g_{aa}(E) = \Delta g_{aa}^{(1)}(E) + \Delta g_{aa}^{(2)}(E) + \cdots\,, \tag{2.49}$$

where the superscript denotes the order in α. If we represent the energy shift as a series in α

$$\Delta E_a = \Delta E_a^{(1)} + \Delta E_a^{(2)} + \cdots\,, \tag{2.50}$$

the formula (2.48) yields

$$\Delta E_a^{(1)} = \frac{1}{2\pi i}\oint_\Gamma dE\,\Delta E\,\Delta g_{aa}^{(1)}(E)\,, \tag{2.51}$$

$$\Delta E_a^{(2)} = \frac{1}{2\pi i}\oint_\Gamma dE\,\Delta E\,\Delta g_{aa}^{(2)}(E) - \left(\frac{1}{2\pi i}\oint_\Gamma dE\,\Delta E\,\Delta g_{aa}^{(1)}(E)\right)\left(\frac{1}{2\pi i}\oint_\Gamma dE\,\Delta g_{aa}^{(1)}(E)\right), \tag{2.52}$$

where $\Delta E \equiv E - E_a^{(0)}$.

Deriving equations (2.44) and (2.48) we assumed that a non-zero photon mass μ is introduced. This allows taking all the cuts outside the contour Γ as well as regularizing the infrared singularities of individual diagrams. In the Feynman gauge, the photon propagator with non-zero photon mass μ is

$$D_{\rho\sigma}(\omega, \mathbf{x}-\mathbf{y}) = -g_{\rho\sigma}\int \frac{d\mathbf{k}}{(2\pi)^3}\,\frac{\exp\left(i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right)}{\omega^2 - \mathbf{k}^2 - \mu^2 + i0} \tag{2.53}$$

or, after integration,

$$D_{\rho\sigma}(\omega, \mathbf{x}-\mathbf{y}) = g_{\rho\sigma}\frac{\exp\left(i\sqrt{\omega^2 - \mu^2 + i0}\,|\mathbf{x}-\mathbf{y}|\right)}{4\pi|\mathbf{x}-\mathbf{y}|}\,, \tag{2.54}$$

where $\mathrm{Im}\sqrt{\omega^2 - \mu^2 + i0} > 0$. $D_{\rho\sigma}(\omega, \mathbf{x}-\mathbf{y})$ is an analytical function of ω in the complex ω plane with cuts beginning at the points $\omega = -\mu + i0$ and $\omega = \mu - i0$ (Fig. 8). The related expressions for the photon propagator with non-zero photon mass in other covariant gauges are presented in [24]. However, since we can put $\mu = 0$ already on an intermediate stage of calculations (see below), we actually do not need any specific expression for the photon propagator with non-zero photon mass. It is sufficient only to assume that in another gauge the photon propagator has the same analytical properties as in the Feynman gauge.

As was noted in the previous subsection, the singularities of the two-time Green function in the complex E plane are defined by the unperturbed Hamiltonian if it is constructed by perturbation theory. In particular, it means that in n-th order of the perturbation theory $g_{aa}(E)$ has poles of all order till $n+1$ at the unperturbed position of the energy level under consideration. Therefore, in calculations by the perturbation theory it is sufficient to consider the photon mass as a very small parameter which provides a separation of the pole from the related cut. At the end of calculations after taking into account a whole gauge invariant set of Feynman diagrams we can put $\mu \to 0$. The possibility of taking the limit $\mu \to 0$ follows, in particular, from the fact that the contour Γ can be drawn continuosly to the point $E = E_a^{(0)}$ (see Fig. 7).

Generally speaking, the energy shift of an excited level derived by formula (2.48) contains an imaginary component which is caused by its instability. This component defines the width of the spectral line in the Lorentz approximation (see sections III F, III G for details).

For practical calculations it is convenient to express the Green function $g_{aa}(E)$ in terms of the Fourier transform of the $2N-$time Green function defined by equation (2.12). By using the identity

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\,\exp\left(i\omega x\right) = \delta(\omega) \tag{2.55}$$

one easily finds (see Appendix C)

$$g_{aa}(E)\delta(E-E') = \frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0 \times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0) \times\langle u_a|G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0)\gamma_1^0\ldots\gamma_N^0|u_a\rangle\,, \tag{2.56}$$

where

$$\langle u_a|G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0)\gamma_1^0\ldots\gamma_N^0|u_a\rangle \equiv \int d\mathbf{x}_1\cdots d\mathbf{x}_N d\mathbf{x}'_1\cdots d\mathbf{x}'_N u_a(\mathbf{x}'_1,...,\mathbf{x}'_N) \times G((p_1'^0,\mathbf{x}'_1),\ldots,(p_N'^0,\mathbf{x}'_N);(p_1^0,\mathbf{x}_1),\ldots,(p_N^0,\mathbf{x}_N)) \times\gamma_1^0\ldots\gamma_N^0 u_a(\mathbf{x}_1,...,\mathbf{x}_N)\,. \tag{2.57}$$

According to equation (2.38) the calculation of the matrix elements in (2.56) is reduced to the calculation of the matrix elements between the one-determinant wave functions

$$u_i = \frac{1}{\sqrt{N!}}\sum_P (-1)^P \psi_{Pi_1}(\mathbf{x}_1)\cdots\psi_{Pi_N}(\mathbf{x}_N)\,, \tag{2.58}$$

$$u_k = \frac{1}{\sqrt{N!}}\sum_P (-1)^P \psi_{Pk_1}(\mathbf{x}_1)\cdots\psi_{Pk_N}(\mathbf{x}_N)\,. \tag{2.59}$$

To simplify the summation procedure over the permutations in (2.56) which arise from the wave functions as well as the Green function $G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0)$, it is convenient to transform equation (2.56) in the following way. Denoting $\overline{G} = G\gamma_1^0\ldots\gamma_N^0$ we can write

$$\overline{G}((p_1'^0,\xi'_1),\ldots,(p_N'^0,\xi'_N);(p_1^0,\xi_1)\ldots,(p_N^0,\xi_N)) = \sum_P (-1)^P \widehat{G}((p'^0_{P1},\xi'_{P1}),\ldots,(p'^0_{PN},\xi'_{PN});(p_1^0,\xi_1),\ldots,(p_N^0,\xi_N))\,, \tag{2.60}$$

where $\xi\equiv(\mathbf{x},\alpha)$ and α is the bispinor index ($\alpha=1,2,3,4$). Substituting (2.60) in (2.56) and using the symmetry of $\widehat{G}$ in respect to electron coordinates, for $g_{ik}(E)=\langle u_i|g(E)|u_k\rangle$ one can obtain (see Appendix D)

$$g_{ik}(E)\delta(E-E') = \frac{2\pi}{i}\sum_P (-1)^P \psi^*_{Pi_1}(\xi'_1)\ldots\psi^*_{Pi_N}(\xi'_N)\int_{-\infty}^{\infty} dp_1^0\ldots dp_N^0 dp_1'^0\ldots dp_N'^0 \times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0) \times\widehat{G}((p_1'^0,\xi'_1),\ldots,(p_N'^0,\xi'_N);(p_1^0,\xi_1),\ldots,(p_N^0,\xi_N)) \times\psi_{k_1}(\xi_1)\ldots\psi_{k_N}(\xi_N)\,, \tag{2.61}$$

where repeated variables $\{\xi\}$ imply integration (the integration over $\mathbf{x}$ and the summation over α). In practical calculations by perturbation theory the formula (2.61) must be employed only for symmetric sets of Feynman diagrams since the symmetry property was used in its derivation.

D. Perturbation theory for degenerate and quasidegenerate levels

Let we are interested in the atomic levels with energies $E_1,...,E_s$ arising from unperturbed degenerate or quasidegenerate levels with energies $E_1^{(0)},...,E_s^{(0)}$. We assume, as usual, that the energy shifts of the levels under consideration or their splitting caused by the interaction are much smaller than the distance to other levels. The unperturbed eigenstates form a s-dimensional subspace Ω. We denote the projector on Ω by

$$P^{(0)} = \sum_{k=1}^{s} P_k^{(0)} = \sum_{k=1}^{s} u_k u_k^\dagger\,, \tag{2.62}$$

where $\{u_k\}_{k=1}^s$ are the unperturbed wave functions which, in a general case, are linear combinations of one-determinant functions (see equation (2.38)). We project the Green function $\mathcal{G}(E)$ on the subspace Ω

$$g(E) = P^{(0)}\mathcal{G}(E)\gamma_1^0 ... \gamma_N^0 P^{(0)}\,, \tag{2.63}$$

where, as in (2.39), the integration over the electron coordinates is implicit. As in the case of a single level, to isolate the poles of $g(E)$ corresponding to the bound states under consideration we introduce a nonzero photon mass μ. We assume that the photon mass μ is larger than the energy distance between the levels under consideration and much smaller than the distance to other levels. In this case we can choose a contour Γ in the complex E plane so that it surrounds all the poles corresponding to the considered states $(E^{(1)}, ...E^{(s)})$ and keeps outside all other singularities including the cuts starting from the lower-lying bound states (see Fig. 9). If, in addition, we neglect the instability of the states under consideration, the spectral representation (see equations (2.24)-(2.34)) gives

$$g(E) = \sum_{k=1}^{s} \frac{\varphi_k \varphi_k^\dagger}{E - E^{(k)}} + \text{ terms that are regular inside } \Gamma\,, \tag{2.64}$$

where

$$\varphi_k = P^{(0)}\Phi_k\,, \qquad \varphi_k^\dagger = \Phi_k^\dagger P^{(0)}\,. \tag{2.65}$$

As in the case of a single level, in the zeroth approximation one easily finds

$$g^{(0)}(E) = \sum_{k=1}^{s} \frac{P_k^{(0)}}{E - E_k^{(0)}}\,. \tag{2.66}$$

We introduce the operators K and P by

$$K \equiv \frac{1}{2\pi i}\oint_\Gamma dE\; E g(E)\,, \tag{2.67}$$

$$P \equiv \frac{1}{2\pi i}\oint_\Gamma dE\; g(E)\,. \tag{2.68}$$

Using equation (2.64) one obtains

$$K = \sum_{i=1}^{s} E^{(i)} \varphi_i \varphi_i^\dagger\,, \tag{2.69}$$

$$P = \sum_{i=1}^{s} \varphi_i \varphi_i^\dagger\,. \tag{2.70}$$

We note here that, generally speaking, the operator P is not a projector (in particular, $P^2 \neq P$). If the perturbation goes to zero, the vectors $\{\varphi_i\}_{i=1}^s$ approach to the correct linearly independent combinations of the vectors $\{u_i\}_{i=1}^s$. Therefore, it is natural to assume that the vectors $\{\varphi_i\}_{i=1}^s$ are also linearly independent. It follows that one can find such vectors $\{v_i\}_{i=1}^s$ that

$$\varphi_i^\dagger v_k = \delta_{ik}\,. \tag{2.71}$$

Indeed, let

$$\varphi_i = \sum_{j=1}^{s} a_{ij} u_j\,, \qquad v_k = \sum_{l=1}^{s} x_{kl} u_l\,. \tag{2.72}$$

The biorthogonality condition (2.71) gives

$$\sum_{j=1}^{s} a_{ij} x_{kj} = \delta_{ik}\,. \tag{2.73}$$

Since the determinant of the matrix $\{a_{ij}\}$ is nonvanishing due to the linear independence of $\{\varphi_i\}_{i=1}^s$, for any fixed $k = 1, ..., s$ the system (2.73) has a unique solution. From (2.69)-(2.71) we have

$$Pv_k = \sum_{i=1}^{s} \varphi_i \varphi_i^\dagger v_k = \varphi_k \,, \tag{2.74}$$

$$Kv_k = \sum_{i=1}^{s} E^{(i)} \varphi_i \varphi_i^\dagger v_k = E^{(k)} \varphi_k \,. \tag{2.75}$$

Hence we obtain the equation for v_k, $E^{(k)}$ [25]

$$Kv_k = E^{(k)} P v_k \,. \tag{2.76}$$

According to (2.71) the vectors v_k are normalized by the condition

$$v_{k'}^\dagger P v_k = \delta_{k'k} \,. \tag{2.77}$$

The solvability of equation (2.76) yields an equation for the atomic energy levels

$$\det\left(K - EP\right) = 0 \,. \tag{2.78}$$

The generalized eigenvalue problem (2.76) with the normalization condition (2.77) can be transformed by the substitution $\psi_k = P^{\frac{1}{2}} v_k$ to the ordinary eigenvalue problem ("Schrödinger-like equation") [29]

$$H\psi_k = E^{(k)} \psi_k \tag{2.79}$$

with the ordinary normalization condition

$$\psi_k^\dagger \psi_{k'} = \delta_{kk'} \,, \tag{2.80}$$

where $H \equiv P^{-\frac{1}{2}}(K)P^{-\frac{1}{2}}$.

The energy levels are determined from the equation

$$\det(H - E) = 0 \,. \tag{2.81}$$

Generally speaking, the energies obtained by this equation contain imaginary components which are due to instability of excited states. In the case when the imaginary components are much smaller than the energy distance between the levels (or the levels have different quantum numbers), they define the widths of the spectral lines in the Lorentz approximation. In the opposite case, when the imaginary components are comparable with the energy distance between the levels which have the same quantum numbers, the spectral line shape depends on the process of the formation of the states under consideration even in the resonance approximation (see sections III F,G for details). In what follows, calculating the energy levels we will neglect the instability of excited states and in equations (2.79), (2.81) will assume $H \equiv (H + H^\dagger)/2$.

The operators K and P are constructed through the formulas (2.67) and (2.68) by perturbation theory

$$K = K^{(0)} + K^{(1)} + K^{(2)} + \cdots \,, \tag{2.82}$$

$$P = P^{(0)} + P^{(1)} + P^{(2)} + \cdots \,, \tag{2.83}$$

where the superscript denotes the order in α. The operator H is

$$H = H^{(0)} + H^{(1)} + H^{(2)} + \cdots \,, \tag{2.84}$$

where

$$H^{(0)} = K^{(0)} \,, \tag{2.85}$$

$$H^{(1)} = K^{(1)} - \frac{1}{2} P^{(1)} K^{(0)} - \frac{1}{2} K^{(0)} P^{(1)} \,, \tag{2.86}$$

$$\begin{aligned} H^{(2)} = {} & K^{(2)} - \frac{1}{2} P^{(2)} K^{(0)} - \frac{1}{2} K^{(0)} P^{(2)} \\ & - \frac{1}{2} P^{(1)} K^{(1)} - \frac{1}{2} K^{(1)} P^{(1)} \\ & + \frac{3}{8} P^{(1)} P^{(1)} K^{(0)} + \frac{3}{8} K^{(0)} P^{(1)} P^{(1)} \\ & + \frac{1}{4} P^{(1)} K^{(0)} P^{(1)} \,. \end{aligned} \tag{2.87}$$

It is evident that in the zeroth order

$$K^{(0)}_{ik} = E^{(0)}_i \delta_{ik}\,, \tag{2.88}$$

$$P^{(0)}_{ik} = \delta_{ik}\,, \tag{2.89}$$

$$H^{(0)}_{ik} = E^{(0)}_i \delta_{ik}\,. \tag{2.90}$$

To derive the equations (2.76)-(2.79) we introduced a non-zero photon mass μ which was assumed to be larger than the energy distance between the levels under consideration and much smaller than the distance to other levels. At the end of calculations after taking into account a whole gauge invariant set of Feynman diagrams we can put $\mu \to 0$. The possibility of taking this limit in the case of quasidegenerate states follows from the fact that the cuts can be drawn to the related poles by a deformation of the contour Γ as shown in Fig. 10.

As in the case of a single level, for practical calculations we express the Green function $g(E)$ in terms of the Fourier transform of the $2N$-time Green function

$$\begin{aligned} g(E)\delta(E-E') = \frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0 ... dp_N^0 dp_1'^0 ... dp_N'^0 \; \delta(E - p_1^0 \cdots - p_N^0)\delta(E' - p_1'^0 \cdots - p_N'^0) \\ \times P^{(0)} G(p_1'^0, ... p_N'^0; p_1^0, ... p_N^0)\gamma_1^0 ... \gamma_N^0 P^{(0)}\,, \end{aligned} \tag{2.91}$$

where $G(p_1'^0, ..., p_N'^0; p_1^0, ..., p_N^0)$ is defined by equation (2.12).

E. Practical calculations

In this section we consider some practical applications of the method in the lowest orders of the perturbation theory. In what follows we will use the notation

$$I(\omega) = e^2 \alpha^\rho \alpha^\sigma D_{\rho\sigma}(\omega)\,. \tag{2.92}$$

In addition we will employ the following symmetry properties of the photon propagator

$$I(\omega) = I(-\omega)\,, \qquad I'(\omega) = -I'(-\omega)\,, \tag{2.93}$$

which, in particular, are valid in the Feynman and Coulomb gauges. Here $I'(\omega) \equiv dI(\omega)/d\omega$.

1. Zeroth order approximation

Let us derive first the formula (2.47) using the Feynman rules for G. According to the equations (2.56)-(2.61) we have

$$\begin{aligned} g_{aa}(E)\delta(E-E') = \frac{2\pi}{i}\sum_P (-1)^P \int d\mathbf{x}_1 \cdots d\mathbf{x}_N d\mathbf{x}'_1 \cdots d\mathbf{x}'_N \\ \times \psi^\dagger_{Pa_1}(\mathbf{x}'_1) \cdots \psi^\dagger_{Pa_N}(\mathbf{x}'_N) \int_{-\infty}^{\infty} dp_1^0 \cdots dp_N^0 dp_1'^0 \cdots dp_N'^0 \\ \times \delta(E - p_1^0 - \cdots - p_N^0)\delta(E' - p_1'^0 - \cdots - p_N'^0) \\ \times \frac{i}{2\pi} S_1(p_1^0, \mathbf{x}'_1, \mathbf{x}_1)\delta(p_1'^0 - p_1^0) \cdots \frac{i}{2\pi} S_N(p_N'^0, \mathbf{x}'_N, \mathbf{x}_N)\delta(p_N'^0 - p_N^0) \\ \times \gamma_1^0 \cdots \gamma_N^0 \psi_{a_1}(\mathbf{x}_1) \cdots \psi_{a_N}(\mathbf{x}_N) \end{aligned} \tag{2.94}$$

$$\begin{aligned} = \frac{2\pi}{i}\int_{-\infty}^{\infty} dp_1^0 \cdots dp_N^0 dp_1'^0 \cdots dp_N'^0 \\ \times \delta(E - p_1^0 - \cdots - p_N^0)\delta(E' - p_1'^0 - \cdots - p_N'^0) \\ \times \frac{i}{2\pi}\frac{1}{p_1^0 - \varepsilon_{a_1} + i0}\delta(p_1'^0 - p_1^0) \cdots \frac{i}{2\pi}\frac{1}{p_N^0 - \varepsilon_{a_N} + i0}\delta(p_N'^0 - p_N^0)\,. \end{aligned} \tag{2.95}$$

Integrating over the energies one easily obtains equation (2.47).

Formal expressions for the energy shift in the case of a one-electron atom (or in the case of an atom with one electron over closed shell) can be derived by various methods. In particular, the Dyson-Schwinger equation can be employed for such a derivation. Therefore, the one-electron system is not the best example to demonstrate the advantages of the method under consideration. However, we start with a detailed description of this simple case since it may serve as the simplest introduction to the technique.

Let us consider first a diagram describing the interaction of a one-electron atom with an external potential $\delta V(\mathbf{x})$ to the first order in $\delta V(\mathbf{x})$ (Fig. 11). According to equation (2.56) we have

$$\begin{aligned}\Delta g^{(1)}_{aa}(E)\delta(E-E') &= \frac{2\pi}{i}\int d\mathbf{x}'d\mathbf{z}d\mathbf{x}\psi^\dagger_a(\mathbf{x}')\frac{i}{2\pi}\sum_{n_1}\frac{\psi_{n_1}(\mathbf{x}')\overline{\psi}_{n_1}(\mathbf{z})}{E'-\varepsilon_{n_1}(1-i0)}\\ &\times\frac{2\pi}{i}\gamma^0\delta V(\mathbf{z})\delta(E'-E)\frac{i}{2\pi}\sum_{n_2}\frac{\psi_{n_2}(\mathbf{z})\overline{\psi}_{n_2}(\mathbf{x})}{E-\varepsilon_{n_2}(1-i0)}\gamma^0\psi_a(\mathbf{x})\\ &= \langle a|\sum_{n_1}\frac{|n_1\rangle\langle n_1|}{E-\varepsilon_{n_1}(1-i0)}\delta V\sum_{n_2}\frac{|n_2\rangle\langle n_2|}{E-\varepsilon_{n_2}(1-i0)}|a\rangle\delta(E'-E)\\ &= \frac{1}{(E-\varepsilon_a)^2}\langle a|\delta V|a\rangle\delta(E'-E). \end{aligned} \tag{2.96}$$

Substituting (2.96) into (2.51) we obtain

$$\begin{aligned}\Delta E^{(0)}_a &= \frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g^{(1)}_{aa}(E)\\ &= \frac{1}{2\pi i}\oint_\Gamma dE\frac{\langle a|\delta V|a\rangle}{E-\varepsilon_a} = \langle a|\delta V|a\rangle\,. \end{aligned} \tag{2.97}$$

In the first order in α the QED corrections are defined by the self energy (SE) (Fig. 12) and the vacuum polarization (VP) (Fig. 13) diagrams. Consider first the SE diagram. One finds

$$\begin{aligned}\Delta g^{(1)}_{aa}(E)\delta(E-E') &= \frac{2\pi}{i}\int d\mathbf{x}'d\mathbf{y}d\mathbf{z}d\mathbf{x}\psi^\dagger_a(\mathbf{x}')\frac{i}{2\pi}\sum_{n_1}\frac{\psi_{n_1}(\mathbf{x}')\overline{\psi}_{n_1}(\mathbf{y})}{E'-\varepsilon_{n_1}(1-i0)}\frac{i}{2\pi}\int_{-\infty}^{\infty}dp^0\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\\ &\times e\gamma^\rho\frac{2\pi}{i}\delta(E'-p^0-\omega)\sum_n\frac{\psi_n(\mathbf{y})\overline{\psi}_n(\mathbf{z})}{p^0-\varepsilon_n(1-i0)}D_{\rho\sigma}(\omega,\mathbf{y}-\mathbf{z})\\ &\times e\gamma^\sigma\frac{2\pi}{i}\delta(p^0+\omega-E)\frac{i}{2\pi}\sum_{n_2}\frac{\psi_{n_2}(\mathbf{z})\overline{\psi}_{n_2}(\mathbf{x})}{E-\varepsilon_{n_2}(1-i0)}\gamma^0\psi_a(\mathbf{x})\\ &= \frac{1}{(E-\varepsilon_a)^2}e^2\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\int d\mathbf{y}d\mathbf{z}\psi^\dagger_a(\mathbf{y})\alpha^\rho\sum_n\frac{\psi_n(\mathbf{y})\overline{\psi}_n(\mathbf{z})}{E-\omega-\varepsilon_n(1-i0)}\\ &\times D_{\rho\sigma}(\omega,\mathbf{y}-\mathbf{z})\alpha^\sigma\psi_a(\mathbf{z})\delta(E'-E)\,, \end{aligned} \tag{2.98}$$

where $\alpha^\rho\equiv\gamma^0\gamma^\rho=(1,\boldsymbol{\alpha})$. Denoting

$$\langle a|\Sigma(E)|b\rangle = \frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_n\frac{\langle an|e^2\alpha^\rho\alpha^\sigma D_{\rho\sigma}(\omega)|nb\rangle}{E-\omega-\varepsilon_n(1-i0)} \tag{2.99}$$

we get

$$\Delta g^{(1)}_{aa}(E) = \frac{\langle a|\Sigma(E)|a\rangle}{(E-\varepsilon_a)^2}\,. \tag{2.100}$$

Substituting (2.100) into (2.51) one obtains

$$\begin{aligned}\Delta E^{(1)}_a &= \frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g^{(1)}_{aa}(E)\\ &= \frac{1}{2\pi i}\oint_\Gamma dE\frac{\langle a|\Sigma(E)|a\rangle}{E-\varepsilon_a} = \langle a|\Sigma(\varepsilon_a)|a\rangle\,. \end{aligned} \tag{2.101}$$

Here we have taken into account the fact that, for a non-zero photon mass μ, $\Delta g(E)$ has isolated poles at $E=\varepsilon_a$ in every order of the perturbation theory. In the final expression one can put $\mu\to 0$.

The expression (2.101) suffers from an ultraviolet divergency and has to be considered together with a counterterm diagram (Fig. 14). Taking into account the counterterm results in a replacement

$$\langle a|\Sigma(\varepsilon_a)|a\rangle \to \langle a|\Sigma_R(\varepsilon_a)|a\rangle = \langle a|(\Sigma(\varepsilon_a)-\gamma^0\delta m)|a\rangle\,. \tag{2.102}$$

The corresponding calculation for the VP diagram (Fig. 13) yields

$$\begin{aligned}\Delta g^{(1)}_{aa}(E)\delta(E-E') = -\frac{2\pi}{i}\int d\mathbf{x}d\mathbf{y}\overline{\psi}_a(\mathbf{x})\frac{i}{2\pi}\frac{1}{E'-\varepsilon_a}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega' \\ \times e\gamma^\rho\frac{2\pi}{i}\delta(E'+\omega'-E)D_{\rho\sigma}(\omega',\mathbf{x}-\mathbf{y})e\frac{2\pi}{i}\delta(\omega') \\ \times\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\mathrm{Tr}\Big[\sum_n\frac{\psi_n(\mathbf{y})\overline{\psi}_n(\mathbf{y})}{\omega-\varepsilon_n(1-i0)}\gamma^\sigma\Big]\frac{i}{2\pi}\frac{1}{E-\varepsilon_a}\psi_a(\mathbf{x})\,.\end{aligned} \tag{2.103}$$

Introducing the VP potential by

$$U_{\rm VP}(\mathbf{x}) = \frac{e^2}{2\pi i}\int d\mathbf{y}\alpha^\rho D_{\rho\sigma}(0,\mathbf{x}-\mathbf{y})\int_{-\infty}^{\infty}d\omega\mathrm{Tr}\Big[\sum_n\frac{\psi_n(\mathbf{y})\psi_n^\dagger(\mathbf{y})}{\omega-\varepsilon_n(1-i0)}\alpha^\sigma\Big] \tag{2.104}$$

one finds

$$\Delta g^{(1)}_{aa}(E) = \frac{\langle a|U_{\rm VP}|a\rangle}{(E-\varepsilon_a)^2} \tag{2.105}$$

and, therefore,

$$\Delta E^{(1)}_a = \langle a|U_{\rm VP}|a\rangle\,. \tag{2.106}$$

In reality, due to a spherical symmetry of the Coulomb potential of the nucleus, only zeroth components of the α matrices contribute to $U_{\rm VP}$,

$$U_{\rm VP}(\mathbf{x}) = \frac{\alpha}{2\pi i}\int d\mathbf{y}\frac{1}{|\mathbf{x}-\mathbf{y}|}\int_{-\infty}^{\infty}d\omega\mathrm{Tr}[G_{\rm C}(\omega,\mathbf{y},\mathbf{y})]\,, \tag{2.107}$$

where

$$G_{\rm C}(\omega,\mathbf{x},\mathbf{y}) = \sum_n\frac{\psi_n(\mathbf{x})\psi_n^\dagger(\mathbf{y})}{\omega-\varepsilon_n(1-i0)} \tag{2.108}$$

is the Coulomb Green function. The expression (2.107) is ultraviolet divergent. The charge renormalization makes it finite.

Let us now consider the combined δV-SE corrections described by Feynman diagrams presented in Fig. 15. For the diagrams "a" and "b" one easily finds

$$\begin{aligned}\Delta g^{(2,a+b)}_{aa}(E) = \frac{1}{(E-\varepsilon_a)^2}\sum_n\langle a|\delta V|n\rangle\frac{1}{E-\varepsilon_n}\langle n|\Sigma(E)|a\rangle \\ +\frac{1}{(E-\varepsilon_a)^2}\sum_n\langle a|\Sigma(E)|n\rangle\frac{1}{E-\varepsilon_n}\langle n|\delta V|a\rangle\,.\end{aligned} \tag{2.109}$$

This contribution is conveniently divided into two parts: *irreducible* ($\varepsilon_n\neq\varepsilon_a$) and *reducible* ($\varepsilon_n=\varepsilon_a$). For the irreducible part one obtains

$$\begin{aligned}\frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g^{(2,a+b,\mathrm{irr})}_{aa}(E) &= \frac{1}{2\pi i}\oint_\Gamma dE\frac{1}{E-\varepsilon_a}\sum_n^{(n\neq a)}\Big[\frac{\langle a|\delta V|n\rangle\langle n|\Sigma(E)|a\rangle}{E-\varepsilon_n} \\ &\quad+\frac{\langle a|\Sigma(E)|n\rangle\langle n|\delta V|a\rangle}{E-\varepsilon_n}\Big] \\ &= \sum_n^{(n\neq a)}\Big[\frac{\langle a|\delta V|n\rangle\langle n|\Sigma(\varepsilon_a)|a\rangle}{\varepsilon_a-\varepsilon_n} \\ &\quad+\frac{\langle a|\Sigma(\varepsilon_a)|n\rangle\langle n|\delta V|a\rangle}{\varepsilon_a-\varepsilon_n}\Big]\end{aligned} \tag{2.110}$$

Here we have taken into account that, due to a spherical symmetry of the Coulomb potential, non-diagonal matrix elements $\langle a|\Sigma(\varepsilon_a)|b\rangle$ are equal to zero if $\varepsilon_a = \varepsilon_b$. The reducible part is

$$\begin{aligned}\frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g_{aa}^{(2,a+b,\mathrm{red})}(E) &= \frac{1}{2\pi i}\oint_\Gamma dE\frac{1}{(E-\varepsilon_a)^2}\Big[\langle a|\delta V|a\rangle\langle a|\Sigma(E)|a\rangle \\ &\quad +\langle a|\Sigma(E)|a\rangle\langle a|\delta V|a\rangle\Big] \\ &= 2\langle a|\delta V|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle\,, \end{aligned} \tag{2.111}$$

where $\Sigma'(\varepsilon_a) \equiv (d\Sigma(E)/dE)_{E=\varepsilon_a}$. The reducible contribution should be considered together with the related contribution from the second term in equation (2.52). Taking into account that

$$\frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g_{aa}^{(1,\delta V)}(E) = \langle a|\delta V|a\rangle \tag{2.112}$$

and

$$\frac{1}{2\pi i}\oint_\Gamma dE\Delta g_{aa}^{(1,\mathrm{SE})}(E) = \frac{1}{2\pi i}\oint_\Gamma dE\frac{\langle a|\Sigma(E)|a\rangle}{(E-\varepsilon_a)^2} = \langle a|\Sigma'(\varepsilon_a)|a\rangle \tag{2.113}$$

we obtain

$$-\Big(\frac{1}{2\pi i}\oint_\Gamma dE(E-\varepsilon_a)\Delta g_{aa}^{(1,\delta V)}(E)\Big)\Big(\frac{1}{2\pi i}\oint_\Gamma dE\Delta g_{aa}^{(1,\mathrm{SE})}(E)\Big) = -\langle a|\delta V|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle\,. \tag{2.114}$$

For the total contribution of the diagrams "a" and "b" one finds

$$\begin{aligned}\Delta E_a^{(2,a+b)} = &\sum_n^{(n\neq a)}\Big[\frac{\langle a|\delta V|n\rangle\langle n|\Sigma(\varepsilon_a)|a\rangle}{\varepsilon_a-\varepsilon_n} + \frac{\langle a|\Sigma(\varepsilon_a)|n\rangle\langle n|\delta V|a\rangle}{\varepsilon_a-\varepsilon_n}\Big] \\ &+\langle a|\delta V|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle\,. \end{aligned} \tag{2.115}$$

For the diagram "c" one obtains

$$\begin{aligned}\Delta g_{aa}^{(2,c)}(E) = &\frac{1}{(E-\varepsilon_a)^2}e^2\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\int d\mathbf{x}\,d\mathbf{y}\,d\mathbf{z}\,\psi_a^\dagger(\mathbf{y})\alpha^\rho\sum_{n_1}\frac{\psi_{n_1}(\mathbf{y})\psi_{n_1}^\dagger(\mathbf{x})}{E-\omega-\varepsilon_{n_1}(1-i0)}\delta V(\mathbf{x}) \\ &\times\sum_{n_2}\frac{\psi_{n_2}(\mathbf{x})\psi_{n_2}^\dagger(\mathbf{z})}{E-\omega-\varepsilon_{n_2}(1-i0)}D_{\rho\sigma}(\omega,\mathbf{y}-\mathbf{z})\alpha^\sigma\psi_a(\mathbf{z})\,. \end{aligned} \tag{2.116}$$

This diagram is irreducible. A simple evaluation yields

$$\begin{aligned}\Delta E_a^{(2,c)} = &e^2\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\int d\mathbf{x}\,d\mathbf{y}\,d\mathbf{z}\psi_a^\dagger(\mathbf{y})\alpha^\rho G_{\mathrm{C}}(\varepsilon_a-\omega,\mathbf{y},\mathbf{x})\delta V(\mathbf{x}) \\ &\times G_{\mathrm{C}}(\varepsilon_a-\omega,\mathbf{x},\mathbf{z})D_{\rho\sigma}(\omega,\mathbf{y}-\mathbf{z})\alpha^\sigma\psi_a(\mathbf{z})\,. \end{aligned} \tag{2.117}$$

The related mass counterterm diagrams (Fig. 16) are accounted for by the replacement $\Sigma \to \Sigma_R = \Sigma - \gamma^0\delta m$ in equation (2.115). This replacement makes the irreducible contribution in equation (2.115) to be finite. As to the reducible contribution, its ultraviolet and infrared divergencies are cancelled with the corresponding divergencies of the vertex contribution given by equation (2.117).

3. Atom with one electron over closed shells

The consideration given above can easily be adopted to the case of an atom with one electron over closed shells by regarding the closed shells as belonging to a new vacuum. The redefinition of the vacuum results in replacing $i0$ with $-i0$ in the electron propagator denominators corresponding to the closed shells. In other words, it means replacing the standard Feynman contour of integration over the electron energy C by a new contour C' (Fig. 17). In this formalism the one-electron radiative corrections are incorporated with the interelectronic-interaction corrections and the energy of the closed shells is considered as the origin of reference. The difference of the integrals along C' and C is

an integral along the contour $C_{\rm int}$. It describes the interaction of the valent electron with the closed shells electrons. Therefore, to find the interelectronic-interaction corrections we have to replace the contour C in the expressions for the one-electron radiative corrections by the contour $C_{\rm int}$. For example, in the case of one electron over the $(1s)^2$ shell in a lithiumlike ion, the first order interelectrinic-interaction corrections are obtained from the formulas for the SE and VP corrections derived above by the replacement

$$\sum_n \frac{|n\rangle\langle n|}{\omega-\varepsilon_n(1-i0)} \to -\frac{2\pi}{i}\delta(\omega-\varepsilon_{1s})\sum_c^{(\varepsilon_c=\varepsilon_{1s})}|c\rangle\langle c|\,. \tag{2.118}$$

As a result of this repalacement, one obtains for the interelectronic-interaction correction

$$\Delta E_a^{(1,{\rm int})} = \sum_c^{(\varepsilon_c=\varepsilon_{1s})}\left[\langle ac|I(0)|ac\rangle - \langle ac|I(\varepsilon_a-\varepsilon_{1s})|ca\rangle\right], \tag{2.119}$$

where $I(\omega)$ is defined by equation(2.92). In [34] this formalism was employed to derive formal expressions for the interelectronic-interaction corrections to the hyperfine splitting in lithiumlike ions.

4. Two-electron atom

Let us consider now the energy shift of a single level (n) in a two-electron atom. In the first order in α, in addition to one-electron SE and VP contributions (Figs. 18,19) we have to consider the one-photon exchange diagram (Fig. 20). Since the derivation of the energy shift from the SE and VP diagrams is easily reduced to the case of a one-electron atom by simple integration over the energy of a disconnected electron propagator, we discuss below only the one-photon exchange diagram.

For simplicity, we assume that the unperturbed wave function of the state under consideration is the one-determinant function

$$u_n(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\sum_P(-1)^P\psi_{Pa}(\mathbf{x_1})\psi_{Pb}(\mathbf{x_2})\,. \tag{2.120}$$

The transition to the general case of a many-determinant function (2.38) causes no problem and can be done in the final expression for the energy shift.

According to equation (2.56), for the one-photon exchange diagram one finds

$$\begin{aligned}\Delta g_{nn}^{(1)} = \Big(\frac{i}{2\pi}\Big)^2\int_{-\infty}^{\infty}dp_1^0dp_1'^0\sum_P(-1)^P\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}\,\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\\ \times\frac{1}{p_1^0-\varepsilon_a+i0}\,\frac{1}{E-p_1^0-\varepsilon_b+i0}\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle\,.\end{aligned} \tag{2.121}$$

Formula (2.51) gives

$$\begin{aligned}\Delta E_n^{(1)} = \frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Big(\frac{i}{2\pi}\Big)^2\int_{-\infty}^{\infty}dp_1^0dp_1'^0\sum_P(-1)^P\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}\\ \times\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\,\frac{1}{p_1^0-\varepsilon_a+i0}\,\frac{1}{E-p_1^0-\varepsilon_b+i0}\\ \times\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle\,,\end{aligned} \tag{2.122}$$

where, as in (2.51), $\Delta E\equiv E-E_n^{(0)}$. Transforming

$$\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}\,\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0} = \frac{1}{\Delta E}\Big(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\Big)\,, \tag{2.123}$$

$$\frac{1}{p_1^0-\varepsilon_a+i0}\,\frac{1}{E-p_1^0-\varepsilon_b+i0} = \frac{1}{\Delta E}\Big(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_b+i0}\Big) \tag{2.124}$$

we obtain

$$\Delta E_n^{(1)} = \frac{1}{2\pi i}\oint_\Gamma dE \frac{1}{\Delta E}\Big\{\Big(\frac{i}{2\pi}\Big)^2 \int_{-\infty}^{\infty} dp_1^0 dp_1'^0 \sum_P (-1)^P \Big(\frac{1}{p_1'^0 - \varepsilon_{Pa} + i0} + \frac{1}{E - p_1'^0 - \varepsilon_{Pb} + i0}\Big)$$
$$\times \Big(\frac{1}{p_1^0 - \varepsilon_a + i0} + \frac{1}{E - p_1^0 - \varepsilon_b + i0}\Big) \langle PaPb|I(p_1'^0 - p_1^0)|ab\rangle \Big\} . \qquad (2.125)$$

The expression in the braces of (2.125) is a regular function of E inside the contour Γ, if the photon mass μ is chosen as indicated above. A direct way to check this fact consists in integrating over p_1^0 and $p_1'^0$ by using the apparent expression for the photon propagator given by equation (2.53). It can also be understood by observing that the integrand in this expression is the sum of terms which contain singularities in p_1^0 ($p_1'^0$) (for real E) from the electron propagators only above or only below the real axis. Therefore, in each term we can vary E in the complex E plane within the contour Γ, keeping the same order of bypassing the singularities in the p_1^0 ($p_1'^0$) integration by moving slightly the contour of the p_1^0 ($p_1'^0$) integration into the complex plane. The branch points of the photon propagators are moved outside the contour Γ due to the non-zero photon mass. However, we do not need to do these proofs since we know the general analytical properties of the Green function $g_{nn}(E)$ in the complex E plane in every order of the perturbation theory (see the related discussion above and Appendix B). According to these properties the function $\Delta g_{nn}^{(1)}(E)$ can have poles at the point $E = E_n^{(0)}$ of order not higher than 2 and, therefore, the expression in the braces of (2.125) is a regular function of E at this point. So, we have to calculate the first order residue at the point $E = E_n^{(0)}$. We stress also that we do not need any apparent form for the analytical continuation of the expression in the braces to the complex E plane since we calculate it only for real E, at the point $E = E_n^{(0)}$, where the present expression is valid. Calculating the E residue we get

$$\Delta E_n^{(1)} = \Big(\frac{i}{2\pi}\Big)^2 \int_{-\infty}^{\infty} dp_1^0 dp_1'^0 \sum_P (-1)^P \Big(\frac{1}{p_1'^0 - \varepsilon_{Pa} + i0} + \frac{1}{-(p_1'^0 - \varepsilon_{Pa}) + i0}\Big)$$
$$\times \Big(\frac{1}{p_1^0 - \varepsilon_a + i0} + \frac{1}{-(p_1^0 - \varepsilon_a) + i0}\Big) \langle PaPb|I(p_1'^0 - p_1^0)|ab\rangle . \qquad (2.126)$$

Taking into account the identity

$$\frac{i}{2\pi}\Big(\frac{1}{x + i0} + \frac{1}{-x + i0}\Big) = \delta(x) \qquad (2.127)$$

we find

$$\Delta E_n^{(1)} = \sum_P (-1)^P \langle PaPb|I(\varepsilon_{Pa} - \varepsilon_a)|ab\rangle . \qquad (2.128)$$

Let us consider now some general remarks to the derivation given above. In order to perform first the integration over E we have separated the singularity in ΔE by employing the identities (2.123) and (2.124). Another way could consist in transforming the left-hand sides of equations (2.123) and (2.124) by the identity

$$\frac{1}{p^0 - \varepsilon_a + i0}\frac{1}{E - p^0 - \varepsilon_b + i0} = \frac{2\pi}{i}\delta(p^0 - \varepsilon_a)\frac{1}{\Delta E}$$
$$+ \frac{1}{p^0 - \varepsilon_a - i0}\frac{1}{E - p^0 - \varepsilon_b + i0} , \qquad (2.129)$$

where we have used equation (2.127). Using this identity allows one to separate contributions singular in $1/\Delta E$ from non-singular ones. The singular contributions result only from the first term in the right-hand side of equation (2.129). It can easily be understood by observing that the second term has both singularities in p^0 (for real E) above the real axis. It follows that the contour of the p^0 integration in the expression for the energy shift can be moved slightly into the complex E plane keeping the same order of bypassing the singularities. It means that we can vary E in the complex E plane within the contour Γ and, therefore, the integrand is a regular function of E within this contour. The identities like (2.129) are very useful for calculations in three- and more electron atoms.

We want also to note that in all cases the order of the singularity in $1/\Delta E$ is quite evident from the type of the diagram under consideration. If the diagram is irreducible, the factors $1/\Delta E$ may come only from the initial and final propagators. In this case the second term in the right-hand side of equation (2.129) does not contribute to the energy shift and, therefore, the derivation of the formal expression for the energy shift becomes trivial. For reducible diagrams the factors $1/\Delta E$ arise also from internal electron propagators.

We can formulate the following simple rule for deriving the energy shift from a certain diagram. Using the identities like (2.123), (2.124) or (2.129) we separate all singularities in $1/\Delta E$ and then integrate over E assuming that the rest is a regular function of E within the contour Γ. As is discussed above, the order of the singularity is quite evident for every specific diagram and it is a simple task to separate the factor $1/\Delta E$ to the correct power. However, if even one separates this factor to a power which is larger or smaller than the real order of the singularity, it is impossible to miss the correct result. In the first case (the power is larger than the real order of the singularity) the result of the calculation remains the same as in the case when one separates the factor $1/\Delta E$ to the correct power. In the second case (the power is smaller than the real order of the singularity) one finds an infinite result ($\sim 1/0$). It means that we should increase the power of the separated singularity and repeat the calculation until we get a finite result.

5. Two-photon exchange diagrams for the ground state of a heliumlike atom

The two-photon exchange diagrams are presented in Fig. 21. Here we derive the energy shift from these diagrams in the case of the ground state of a heliumlike atom. The case of an arbitrary state of a two-electron atom is considered in detail in [32]. The wave function of the ground state is given by

$$u_1(\mathbf{x}_1,\mathbf{x}_2)=\frac{1}{\sqrt{2}}\sum_P(-1)^P\psi_{Pa}(\mathbf{x}_1)\psi_{Pb}(\mathbf{x}_2) \tag{2.130}$$

The unperturbed energy is $E_1^{(0)}=\varepsilon_a+\varepsilon_b$, where $\varepsilon_a=\varepsilon_b$.

Consider first the two-photon ladder diagram (Fig. 21a). For the first term in (2.52) we have

$$\begin{aligned}\Delta E^{(2)}_{\rm lad}=&\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\sum_P(-1)^P\Big(\frac{i}{2\pi}\Big)^3\int_{-\infty}^{\infty}dp_1^0dp_1'^0d\omega\\
&\times\sum_{n_1n_2}\langle PaPb|I(p_1'^0-\omega)|n_1n_2\rangle\langle n_1n_2|I(\omega-p_1^0)|ab\rangle\\
&\times\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\frac{1}{\omega-\varepsilon_{n_1}(1-i0)}\\
&\times\frac{1}{E-\omega-\varepsilon_{n_2}(1-i0)}\frac{1}{p_1^0-\varepsilon_a+i0}\frac{1}{E-p_1^0-\varepsilon_b+i0}\,.\end{aligned} \tag{2.131}$$

Let us divide this contribution into irreducible ($\varepsilon_{n_1}+\varepsilon_{n_2}\neq\varepsilon_a+\varepsilon_b$) and reducible ($\varepsilon_{n_1}+\varepsilon_{n_2}=\varepsilon_a+\varepsilon_b$) parts

$$\Delta E^{(2)}_{\rm lad}=\Delta E^{(2,{\rm irred})}_{\rm lad}+\Delta E^{(2,{\rm red})}_{\rm lad}\,. \tag{2.132}$$

Using the identities (2.123) and (2.124) we obtain for the irreducible part

$$\begin{aligned}\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g^{(2,{\rm irred})}_{11}(E)=&\frac{1}{2\pi i}\oint_\Gamma dE\frac{1}{\Delta E}\Big\{\sum_P(-1)^P\Big(\frac{i}{2\pi}\Big)^3\int_{-\infty}^{\infty}dp_1^0dp_1'^0d\omega\\
&\times\sum_{n_1,n_2}^{\varepsilon_{n_1}+\varepsilon_{n_2}\neq\varepsilon_a+\varepsilon_b}\langle PaPb|I(p_1'^0-\omega)|n_1n_2\rangle\langle n_1n_2|I(\omega-p_1^0)|ab\rangle\\
&\times\Big(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\Big)\\
&\times\frac{1}{\omega-\varepsilon_{n_1}(1-i0)}\frac{1}{E-\omega-\varepsilon_{n_2}(1-i0)}\\
&\times\Big(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_b+i0}\Big)\Big\}\,.\end{aligned} \tag{2.133}$$

The expression in the braces of (2.133) is a regular function of E inside the contour Γ if the photon mass μ is chosen as indicated above (if it is not so, we would get an infinite result; see the related discussion in the previous subsection). Calculating the E residue we find

$$\Delta E^{(2,\mathrm{irred})}_{\mathrm{lad}} = \sum_P (-1)^P \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{n_1,n_2}^{\varepsilon_{n_1}+\varepsilon_{n_2}\neq\varepsilon_a+\varepsilon_b} \langle PaPb|I(\varepsilon_{Pa}-\omega)|n_1n_2\rangle$$
$$\times\langle n_1n_2|I(\omega-\varepsilon_a)|ab\rangle \frac{1}{\omega-\varepsilon_{n_1}(1-i0)}\,\frac{1}{E_1^{(0)}-\omega-\epsilon_{n_2}(1-i0)}\,. \tag{2.134}$$

This derivation shows that the energy shift from an irreducible diagram is obtained by evaluation of the "usual S-matrix" element. For the numerical evaluation of (2.134) it is convenient to rotate the contour of the integration in the complex ω plane [65].

For the reducible contribution we have

$$\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g^{(2,\mathrm{red})}_{11}(E) = \frac{1}{2\pi i}\oint_\Gamma dE\frac{1}{(\Delta E)^2}\Big\{\sum_P(-1)^P\Big(\frac{i}{2\pi}\Big)^3\int_{-\infty}^{\infty} dp_1^0dp_1'^0d\omega$$
$$\times\sum_{n_1,n_2}^{\varepsilon_{n_1}+\varepsilon_{n_2}=\varepsilon_a+\varepsilon_b}\langle PaPb|I(p_1'^0-\omega)|n_1n_2\rangle\langle n_1n_2|I(\omega-p_1^0)|ab\rangle$$
$$\times\Big(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\Big)$$
$$\times\Big(\frac{1}{\omega-\varepsilon_{n_1}+i0}+\frac{1}{E-\omega-\varepsilon_{n_2}+i0)}\Big)$$
$$\times\Big(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_b+i0}\Big)\Big\}\,. \tag{2.135}$$

The expression in the braces of (2.135) is a regular function inside the contour Γ. Calculating the E residue and taking into account that $\varepsilon_a=\varepsilon_b$ we get

$$\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g^{(2,\mathrm{red})}_{11}(E) = -\frac{i}{2\pi}\sum_P(-1)^P\sum_{n_1,n_2}^{\varepsilon_{n_1}+\varepsilon_{n_2}=2\varepsilon_a}\Big\{\int_{-\infty}^{\infty}dp_1'^0\langle PaPb|I(p_1'^0-\varepsilon_a)|n_1n_2\rangle$$
$$\times\langle n_1n_2|I(0)|ab\rangle\frac{1}{(\varepsilon_a-p_1'^0+i0)^2}+\int_{-\infty}^{\infty}dp_1^0\langle PaPb|I(0)|n_1n_2\rangle$$
$$\times\langle n_1n_2|I(\varepsilon_a-p_1^0)|ab\rangle\frac{1}{(\varepsilon_a-p_1^0+i0)^2}$$
$$+\int_{-\infty}^{\infty}d\omega\langle PaPb|I(\varepsilon_a-\omega)|n_1n_2\rangle$$
$$\times\langle n_1n_2|I(\omega-\varepsilon_a)|ab\rangle\frac{1}{(\varepsilon_a-\omega+i0)^2}\Big\}\,. \tag{2.136}$$

This contribution should be considered together with the second term in equation (2.52). As was obtained above, the first factor in this term is

$$\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g^{(1)}_{11}(E) = \sum_P(-1)^P\langle PaPb|I(0)|ab\rangle\,. \tag{2.137}$$

A simple calculation of the second factor yields

$$\frac{1}{2\pi i}\oint_\Gamma dE\Delta g^{(1)}_{11}(E) = \frac{1}{2\pi i}\oint_\Gamma dE\frac{1}{(\Delta E)^2}\Big\{\Big(\frac{i}{2\pi}\Big)^2\int_{-\infty}^{\infty}dp_1^0dp_1'^0$$
$$\times\sum_P(-1)^P\Big(\frac{1}{p_1'^0-\varepsilon_a+i0}+\frac{1}{E-p_1'^0-\varepsilon_a+i0}\Big)$$
$$\times\Big(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_a+i0}\Big)\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle$$
$$=-\frac{i}{2\pi}\sum_P(-1)^P\Big\{\int_{-\infty}^{\infty}dp_1'^0\frac{1}{(p_1'^0-\varepsilon_a-i0)^2}\langle PaPb|I(p_1'^0-\varepsilon_a)|ab\rangle$$
$$+\int_{-\infty}^{\infty}dp_1^0\frac{1}{(p_1^0-\varepsilon_a-i0)^2}\langle PaPb|I(p_1^0-\varepsilon_a)|ab\rangle\Big\}\,. \tag{2.138}$$

For the total reducible contribution one obtains

$$\Delta E^{(2,\mathrm{red})}_{\mathrm{lad}} = \frac{1}{2\pi i}\oint_\Gamma dE\,\Delta E\,\Delta g^{(2,\mathrm{red})}_{11}(E) - \left(\frac{1}{2\pi i}\oint_\Gamma dE\,\Delta E\,\Delta g^{(1)}_{11}(E)\right)\left(\frac{1}{2\pi i}\oint_\Gamma dE\,\Delta g^{(1)}_{11}(E)\right)$$
$$= -\sum_P (-1)^P \sum_{n_1,n_2}^{\varepsilon_{n_1}+\varepsilon_{n_2}=2\varepsilon_a} \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \langle PaPb|I(\omega-\varepsilon_a)|n_1n_2\rangle$$
$$\times\langle n_1n_2|I(\omega-\varepsilon_a)|ab\rangle \frac{1}{(\omega-\varepsilon_a-i0)^2}\,. \tag{2.139}$$

A similar calculation of the two-photon crossed-ladder diagram (Fig. 21b) gives

$$\Delta E^{(2)}_{\mathrm{cross}} = \sum_P (-1)^P \sum_{n_1,n_2} \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \langle Pan_2|I(\omega-\varepsilon_a)|n_1b\rangle\langle n_1Pb|I(\omega-\varepsilon_a)|an_2\rangle$$
$$\times \frac{1}{\omega-\varepsilon_{n_1}(1-i0)}\frac{1}{\omega-\varepsilon_{n_2}(1-i0)}\,. \tag{2.140}$$

The contribution $\Delta E^{(2,\mathrm{red})}_{\mathrm{lad}}$ contains an infrared divergent term which is cancelled by a related term ($\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a$) from the contribution $\Delta E^{(2)}_{\mathrm{cross}}$. In the individual contributions the infrared singularities are regularized by a non-zero photon mass μ. If the ladder and crossed-ladder contributions are united by the common ω-integration, the integral is convergent and we can put $\mu\to 0$ before the integration over ω (see [32] for details). However, to show how the calculation for a non-zero photon mass can be performed, let us calculate the reducible contribution for a finite μ. We have to calculate the integral

$$I_1 = \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{\exp\left[i\sqrt{\omega^2-\mu^2+i0}\,(r_{12}+r_{34})\right]}{r_{12}r_{34}}\frac{1}{(\omega-i0)^2}\,. \tag{2.141}$$

Using the identity

$$\exp\left[i\sqrt{\omega^2-\mu^2+i0}\,r\right] = -\frac{2}{\pi}\int_0^\infty dk k\frac{\sin(kr)}{(\omega^2-k^2-\mu^2+i0)} \tag{2.142}$$

we obtain

$$I_1 = -\frac{2}{\pi}\frac{i}{2\pi}\frac{1}{r_{12}r_{34}}\int_{-\infty}^{\infty} d\omega\int_0^\infty dk k\frac{\sin(k(r_{12}+r_{34}))}{(\omega^2-k^2-\mu^2+i0)}\frac{1}{(\omega-i0)^2}\,. \tag{2.143}$$

Decomposing the denominator

$$\omega^2-k^2-\mu^2+i0 = (\omega-\sqrt{k^2+\mu^2}+i0)(\omega+\sqrt{k^2+\mu^2}-i0) \tag{2.144}$$

and integrating over ω one finds

$$I_1 = -\frac{1}{\pi}\frac{1}{r_{12}r_{34}}\int_0^\infty dk\,k\frac{\sin(k(r_{12}+r_{34}))}{(k^2+\mu^2)^{3/2}}\,. \tag{2.145}$$

According to Ref. [66] the last integral is

$$I_1 = -\frac{1}{\pi}\frac{r_{12}+r_{34}}{r_{12}r_{34}}K_0[\mu(r_{12}+r_{34})]\,, \tag{2.146}$$

where

$$K_0(z) = -\log(z/2)\sum_{k=0}^\infty \frac{(z/2)^{2k}}{(k!)^2} + \sum_{k=0}^\infty \frac{z^{2k}}{2^{2k}(k!)^2}\psi(k+1)\,. \tag{2.147}$$

Considering $\mu\to 0$ we find

$$\Delta E^{(2,\mathrm{red})}_{\mathrm{lad}} = -\frac{\alpha^2}{\pi}\sum_P (-1)^P \int d\mathbf{x}_1\cdots\mathbf{x}_4 \overline{\psi}_{Pa}(\mathbf{x}_3)\overline{\psi}_{Pb}(\mathbf{x}_4)\gamma_3^\rho\gamma_4^\sigma$$
$$\times \sum_{n_1,n_2}^{\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a} \psi_{n_1}(\mathbf{x}_3)\overline{\psi}_{n_1}(\mathbf{x}_1)\psi_{n_2}(\mathbf{x}_4)\overline{\psi}_{n_2}(\mathbf{x}_2)\gamma_1^\lambda\gamma_2^\nu\Big(\frac{1}{r_{12}}+\frac{1}{r_{34}}\Big)$$
$$\times[\log(r_{12}+r_{34})+\log\mu-\log 2-\psi(1)]g_{\rho\sigma}g_{\lambda\nu}\psi_a(\mathbf{x}_1)\psi_b(\mathbf{x}_2)\,. \qquad (2.148)$$

The corresponding contribution ($\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a$) from the crossed-ladder diagram is calculated in the same way. The sum of the reducible contribution of the ladder diagram and the related contribution of the crossed-ladder diagram is [25]

$$\Delta E^{(2,\mathrm{infr})} = -\frac{\alpha^2}{\pi}\sum_P (-1)^P \sum_{n_1,n_2}^{\varepsilon_{n_1}=\varepsilon_{n_2}=\varepsilon_a} \int d\mathbf{x}_1\cdots\mathbf{x}_4 \overline{\psi}_{Pa}(\mathbf{x}_3)\overline{\psi}_{Pb}(\mathbf{x}_4)\gamma_3^\rho\gamma_4^\sigma$$
$$\times\psi_{n_1}(\mathbf{x}_3)\overline{\psi}_{n_1}(\mathbf{x}_1)\psi_{n_2}(\mathbf{x}_4)\overline{\psi}_{n_2}(\mathbf{x}_2)\gamma_1^\lambda\gamma_2^\nu$$
$$\times\Big[g_{\rho\sigma}g_{\lambda\nu}\Big(\frac{1}{r_{12}}+\frac{1}{r_{34}}\Big)\log(r_{12}+r_{34})$$
$$-g_{\rho\nu}g_{\sigma\lambda}\Big(\frac{1}{r_{14}}+\frac{1}{r_{23}}\Big)\log(r_{14}+r_{23})\Big]\psi_a(\mathbf{x}_1)\psi_b(\mathbf{x}_2)\,. \qquad (2.149)$$

The terms containing the factor $\log\mu-\log 2-\psi(1)$ have cancelled each other.

6. Qusidegenerate states

Let us now consider some applications of the method for the case of quasidegenerate states. This case arises, for instance, if one is interested in the energies of $(1s2p_{1/2})_1$ and $(1s2p_{3/2})_1$ states of a heliumlike ion. These states are strongly mixed for low and middle Z and, therefore, must be treated as quasidegenerate. It means that the off-diagonal matrix elements of the energy operator H between these states have to be taken into account. The unperturbed wave functions are written as

$$u_i(\mathbf{x}_1,\mathbf{x}_2) = \sum_{m_{i_1}m_{i_2}} \langle j_{i_1}m_{i_1}j_{i_2}m_{i_2}|JM\rangle \frac{1}{\sqrt{2}}\sum_P (-1)^P\psi_{Pi_1}(\mathbf{x}_1)\psi_{Pi_2}(\mathbf{x}_2)\,, \qquad (2.150)$$

where J is the total angular momentum and M is its projection. However, in what follows, to compactify the formulas we will construct the matrix elements of H between the one-determinant wave functions

$$u_i(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\sum_P (-1)^P\psi_{Pi_1}(\mathbf{x}_1)\psi_{Pi_2}(\mathbf{x}_2)\,. \qquad (2.151)$$

The transition to the wave functions defined by equation (2.150) can easily be accomplished in the final formulas.

First we consider the contribution from the one-photon exchange diagram. To derive the formulas for $H^{(1)}_{ik}$ we will assume that $E^{(0)}_i \neq E^{(0)}_k$. However, all the final formulas remain to be valid also for the case $E^{(0)}_i = E^{(0)}_k$ which was considered in detail above. According to the Feynman rules and the definition of $g(E)$, the contribution of the one-photon exchange diagram to $g^{(1)}(E)$ is

$$g^{(1)}_{ik}(E) = \Big(\frac{i}{2\pi}\Big)^2\int_{-\infty}^{\infty} dp_1^0 dp_1'^0 \sum_P (-1)^P \frac{1}{p_1'^0-\varepsilon_{Pi_1}+i0}\frac{1}{E-p_1'^0-\varepsilon_{Pi_2}+i0}$$
$$\times\frac{1}{p_1^0-\varepsilon_{k_1}+i0}\frac{1}{E-p_1^0-\varepsilon_{k_2}+i0}\langle Pi_1Pi_2|I(p_1'^0-p_1^0)|k_1k_2\rangle\,. \qquad (2.152)$$

Using the identities (2.123) and (2.124) we obtain

$$K^{(1)}_{ik} = \frac{1}{2\pi i}\oint_\Gamma dE \frac{E}{(E-E^{(0)}_i)(E-E^{(0)}_k)}\Big\{\Big(\frac{i}{2\pi}\Big)^2\int_{-\infty}^{\infty} dp_1^0 dp_1'^0\sum_P(-1)^P$$
$$\times\Big(\frac{1}{p_1'^0-\varepsilon_{Pi_1}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pi_2}+i0}\Big)\Big(\frac{1}{p_1^0-\varepsilon_{k_1}+i0}+\frac{1}{E-p_1^0-\varepsilon_{k_2}+i0}\Big)$$
$$\times\langle Pi_1Pi_2|I(p_1'^0-p_1^0)|k_1k_2\rangle\Big\}\,. \qquad (2.153)$$

The expression in the braces of (2.153) is a regular function of E inside the contour Γ, if the photon mass μ is chosen as indicated above. Calculating the E residues and taking into account the identity (2.127) we obtain

$$K_{ik}^{(1)} = \frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1^0 \sum_P (-1)^P \frac{E_i^{(0)}\langle Pi_1Pi_2|I(\varepsilon_{Pi_1}-p_1^0)|k_1k_2\rangle}{E_i^{(0)}-E_k^{(0)}}$$
$$\times\Big(\frac{1}{p_1^0-\varepsilon_{k_1}+i0}+\frac{1}{E_i^{(0)}-p_1^0-\varepsilon_{k_2}+i0}\Big)$$
$$+\frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1'^0 \sum_P (-1)^P \frac{E_k^{(0)}\langle Pi_1Pi_2|I(p_1'^0-\varepsilon_{k_1})|k_1k_2\rangle}{E_k^{(0)}-E_i^{(0)}}$$
$$\times\Big(\frac{1}{p_1'^0-\varepsilon_{Pi_1}+i0}+\frac{1}{E_k^{(0)}-p_1'^0-\varepsilon_{Pi_2}+i0}\Big)\,. \tag{2.154}$$

In the same way we find

$$P_{ik}^{(1)} = \frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1^0 \sum_P (-1)^P \frac{\langle Pi_1Pi_2|I(\varepsilon_{Pi_1}-p_1^0)|k_1k_2\rangle}{E_i^{(0)}-E_k^{(0)}}$$
$$\times\Big(\frac{1}{p_1^0-\varepsilon_{k_1}+i0}+\frac{1}{E_i^{(0)}-p_1^0-\varepsilon_{k_2}+i0}\Big)$$
$$+\frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1'^0 \sum_P (-1)^P \frac{\langle Pi_1Pi_2|I(p_1'^0-\varepsilon_{k_1})|k_1k_2\rangle}{E_k^{(0)}-E_i^{(0)}}$$
$$\times\Big(\frac{1}{p_1'^0-\varepsilon_{Pi_1}+i0}+\frac{1}{E_k^{(0)}-p_1'^0-\varepsilon_{Pi_2}+i0}\Big)\,. \tag{2.155}$$

Symmetrizing equations (2.154) and (2.155) in respect to both electrons we transform them to the form

$$K_{ik}^{(1)} = \sum_P (-1)^P \Big\{ \frac{1}{2}[\langle Pi_1Pi_2|I(\Delta_1)|k_1k_2\rangle + \langle Pi_1Pi_2|I(\Delta_2)|k_1k_2\rangle]$$
$$-\frac{(E_i^{(0)}+E_k^{(0)})}{2}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\langle Pi_1Pi_2|I(\omega)|k_1k_2\rangle$$
$$\times\Big[\frac{1}{(\omega+\Delta_1-i0)(\omega-\Delta_2-i0)}+\frac{1}{(\omega+\Delta_2-i0)(\omega-\Delta_1-i0)}\Big] \Big\}\,, \tag{2.156}$$

$$P_{ik}^{(1)} = -\sum_P (-1)^P \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\langle Pi_1Pi_2|I(\omega)|k_1k_2\rangle$$
$$\times\Big[\frac{1}{(\omega+\Delta_1-i0)(\omega-\Delta_2-i0)}+\frac{1}{(\omega+\Delta_2-i0)(\omega-\Delta_1-i0)}\Big]\,, \tag{2.157}$$

where $\Delta_1 = \varepsilon_{Pi_1}-\varepsilon_{k_1}$ and $\Delta_2 = \varepsilon_{Pi_2}-\varepsilon_{k_2}$. Substituting (2.156), (2.157) into (2.86), we get [31,67]

$$H_{ik}^{(1)} = \frac{1}{2}\sum_P (-1)^P[\langle Pi_1Pi_2|I(\Delta_1)|k_1k_2\rangle + \langle Pi_1Pi_2|I(\Delta_2)|k_1k_2\rangle]\,. \tag{2.158}$$

Let us now consider the contribution to H from the combined δV - interelectronic interaction diagrams presented in Fig. 22. For simplicity, we will assume that δV is a spherically-symmetric potential. In the case under consideration, the simplest way to derive the formulas for $H_{ik}^{(2)}$ consists in using the fact that these diagrams can be obtained as the first order correction in δV to the one-photon exchange contribution derived above. So, the contribution from these diagrams can be obtained by the following replacements in equation (2.158)

$$|k_1\rangle \to |k_1\rangle + \delta|k_1\rangle\,, \tag{2.159}$$
$$|k_2\rangle \to |k_2\rangle + \delta|k_2\rangle\,, \tag{2.160}$$

$$|Pi_1\rangle \to |Pi_1\rangle + \delta|Pi_1\rangle\,, \tag{2.161}$$
$$|Pi_2\rangle \to |Pi_2\rangle + \delta|Pi_2\rangle\,, \tag{2.162}$$
$$I(\varepsilon_a - \varepsilon_b) \to I(\varepsilon_a + \delta\varepsilon_a - \varepsilon_b - \delta\varepsilon_b)\,, \tag{2.163}$$

where, to first order in δV,

$$\delta\varepsilon_a = \langle a|\delta V|a\rangle\,, \tag{2.164}$$
$$\delta|a\rangle = \sum_n^{\varepsilon_n\neq\varepsilon_a} \frac{|n\rangle\langle n|\delta V|a\rangle}{\varepsilon_a - \varepsilon_n}\,. \tag{2.165}$$

Here we have taken into account that, due to the spherical symmetry of δV, $\langle n|\delta V|a\rangle = 0$ if $\varepsilon_n = \varepsilon_a$ and $|n\rangle \neq |a\rangle$. Decomposing the modified expression for the one-photon exchange diagram to the first order in δV we find that the total correction is the sum of the irreducible and reducible parts

$$H_{ik}^{(2)} = H_{ik}^{(2,\mathrm{irred})} + H_{ik}^{(2,\mathrm{red})}\,, \tag{2.166}$$

where

$$\begin{aligned} H_{ik}^{(2,\mathrm{irred})} = \frac{1}{2}\sum_P (-1)^P [&\langle \delta P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|k_1 k_2\rangle \\ &+\langle P i_1 \delta P i_2|I(\Delta_1) + I(\Delta_2)|k_1 k_2\rangle \\ &+\langle P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|\delta k_1 k_2\rangle \\ &+\langle P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|k_1 \delta k_2\rangle] \end{aligned} \tag{2.167}$$

and

$$\begin{aligned} H_{ik}^{(2,\mathrm{red})} = \frac{1}{2}\sum_P (-1)^P \{&[\langle P i_1|\delta V|P i_1\rangle - \langle k_1|\delta V|k_1\rangle]\langle P i_1 P i_2|I'(\Delta_1)|k_1 k_2\rangle \\ &+[\langle P i_2|\delta V|P i_2\rangle - \langle k_2|\delta V|k_2\rangle]\langle P i_1 P i_2|I'(\Delta_2)|k_1 k_2\rangle\}\,. \end{aligned} \tag{2.168}$$

Equations (2.167) and (2.168) provide the matrix elements between the one-determinant wave functions defined by equation (2.151). To get the matrix elements between the wave functions defined by equation (2.150), we have to multiply these equations with the Clebsch-Gordan coefficients and to sum over projections of the one-electron angular momenta.

The expression for $H_{ik}^{(2)}$ can also be derived by the direct application of the TTGF method. It can easily be done in the same way as for the one-photon exchange diagram. However, we note that this derivation yields a formula for $H_{ik}^{(2)}$ which is slightly different from the expression given above. In particular, for the irreducible contribution one finds

$$\begin{aligned} H_{ik}^{(2,\mathrm{irred})} = \frac{1}{2}\sum_P (-1)^P [&\langle \delta P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|k_1 k_2\rangle \\ &+\langle P i_1 \delta P i_2|I(\Delta_1) + I(\Delta_2)|k_1 k_2\rangle \\ &+\langle P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|\delta k_1 k_2\rangle \\ &+\langle P i_1 P i_2|I(\Delta_1) + I(\Delta_2)|k_1 \delta k_2\rangle] \\ &+\Delta H_{ik}^{(2,\mathrm{irred})}\,, \end{aligned} \tag{2.169}$$

where

$$\begin{aligned} \Delta H_{ik}^{(2,\mathrm{irred})} = \frac{1}{2}(E_i^{(0)} - E_k^{(0)})\sum_P (-1)^P \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \Big\{ &\frac{\langle \delta P i_1 P i_2|I(\omega - \varepsilon_{P i_1})|k_1 k_2\rangle}{(\omega - \varepsilon_{k_1} + i0)(E_i^{(0)} - \omega - \varepsilon_{k_2} - i0)} \\ &+\frac{\langle P i_1 \delta P i_2|I(\omega - \varepsilon_{P i_1})|k_1 k_2\rangle}{(\omega - \varepsilon_{k_1} - i0)(E_i^{(0)} - \omega - \varepsilon_{k_2} + i0)} \\ &-\frac{\langle P i_1 P i_2|I(\omega - \varepsilon_{k_1})|\delta k_1 k_2\rangle}{(\omega - \varepsilon_{P i_1} + i0)(E_k^{(0)} - \omega - \varepsilon_{P i_2} - i0)} \end{aligned}$$

$$
\begin{aligned}
&- \frac{\langle Pi_1 Pi_2|I(\omega-\varepsilon_{k_1})|k_1\delta k_2\rangle}{(\omega-\varepsilon_{Pi_1}-i0)(E_k^{(0)}-\omega-\varepsilon_{Pi_2}+i0)} \\
&+ \sum_n^{n\neq k_1} \frac{\langle Pi_1 Pi_2|I(\omega-\varepsilon_{Pi_1})|nk_2\rangle\langle n|\delta V|k_1\rangle}{(\omega-\varepsilon_{k_1}-i0)(E_i^{(0)}-\omega-\varepsilon_{k_2}+i0)(\omega-\varepsilon_n(1-i0))} \\
&+ \sum_n^{n\neq k_2} \frac{\langle Pi_1 Pi_2|I(\omega-\varepsilon_{Pi_1})|k_1n\rangle\langle n|\delta V|k_2\rangle}{(\omega-\varepsilon_{k_1}+i0)(E_i^{(0)}-\omega-\varepsilon_{k_2}-i0)(E_i^{(0)}-\omega-\varepsilon_n(1-i0))} \\
&- \sum_n^{n\neq Pi_1} \frac{\langle Pi_1|\delta V|n\rangle\langle nPi_2|I(\omega-\varepsilon_{k_1})|k_1k_2\rangle}{(\omega-\varepsilon_{Pi_1}-i0)(E_k^{(0)}-\omega-\varepsilon_{Pi_2}+i0)(\omega-\varepsilon_n(1-i0))} \\
&- \sum_n^{n\neq Pi_2} \frac{\langle Pi_2|\delta V|n\rangle\langle Pi_1n|I(\omega-\varepsilon_{k_1})|k_1k_2\rangle}{(\omega-\varepsilon_{Pi_1}+i0)(E_k^{(0)}-\omega-\varepsilon_{Pi_2}-i0)(E_k^{(0)}-\omega-\varepsilon_n(1-i0))}\Big\}\,. \qquad (2.170)
\end{aligned}
$$

The term $\Delta H_{ik}^{(2,\mathrm{irred})}$ goes to zero if $E_i^{(0)} \to E_k^{(0)}$. The expressions (2.167) and (2.169) differ by the term $\Delta H_{ik}^{(2,\mathrm{irred})}$ which can be represented as

$$
\Delta H_{ik}^{(2,\mathrm{irred})} = (E_i^{(0)} - E_k^{(0)}) O_{ik}^{(2)}. \qquad (2.171)
$$

Here $O^{(2)}$ is an operator of the second order in the perturbation parameter which we denote by λ (for simplicity, we assume here that δV and the interelectronic-interaction operator $I(\omega)$ are characterized by the same perturbation parameter). This fact can be understood by observing that the integrand in (2.170) is the sum of terms which contain singularities from the external electron propagators only above or below of the real axis and, therefore, integrating over ω cannot result in appearing contributions $\sim 1/(E_i^{(0)} - E_k^{(0)})$ which could compensate the factor $(E_i^{(0)} - E_k^{(0)})$ (in particular, it means that $O_{ik}^{(2)}$ remains finite when $E_i^{(0)} \to E_k^{(0)}$). It can be shown that the term $\Delta H_{ik}^{(2,\mathrm{irred})}$ contributes only to the third and higher orders in λ and, therefore, can be omitted if we restrict our calculations to the second order in λ. Let us prove this fact for the case of two quasidegenerate levels. In this case the energy levels are determined from the equation

$$
(E - H_{11})(E - H_{22}) - H_{12}H_{21} = 0 \qquad (2.172)
$$

which yields

$$
E_{1,2} = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4H_{12}H_{21}}\,. \qquad (2.173)
$$

If $E_1 - E_2 \sim \lambda$, the prove of the statement is evident. If $E_1 - E_2 \gg \lambda$, the contribution of the second order off-diagonal matrix elements is given by

$$
\Delta E_{1,2} \approx \pm(H_{12}^{(2)}H_{21}^{(1)} + H_{12}^{(1)}H_{21}^{(2)})/(E_1^{(0)} - E_2^{(0)})\,. \qquad (2.174)
$$

From this equation one finds that the terms $\sim (E_i^{(0)} - E_k^{(0)})O_{ik}^{(2)}$ in $H_{ik}^{(2)}$ contribute only to the third and higher orders in λ.

In Ref. [68] the TTGF method is employed to derive formulas for the self-energy screening diagrams in the case of quasidegenerate states of a heliumlike atom.

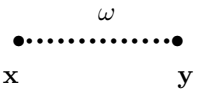
7. Nuclear recoil corrections

So far we considered the nucleus as a sourse of the external Coulomb field V_{C}. This consideration corresponds to the approximation of the infinite nucleus mass. However, high precision calculations of the energy levels in high-Z few-electron atoms must include also the nuclear recoil corrections to first order in m/M (M is the nucleas mass) and to zeroth order in α (but to all orders in αZ). As was shown in [37], these corrections can be included in calculations of the energy levels by adding to the standard Hamiltonian of the electron-positron field interacting with the quantized electromagnetic field and with the Coulomb field of the nuceus V_{C}, taken in the Coulomb gauge, the following term

$$H_M = \frac{1}{2M}\int d\mathbf{x}\psi^\dagger(\mathbf{x})(-i\nabla_\mathbf{x})\psi(\mathbf{x})\int d\mathbf{y}\psi^\dagger(\mathbf{y})(-i\nabla_\mathbf{y})\psi(\mathbf{y})$$
$$-\frac{eZ}{M}\int d\mathbf{x}\psi^\dagger(\mathbf{x})(-i\nabla_\mathbf{x})\psi(\mathbf{x})\mathbf{A}(0)+\frac{e^2Z^2}{2M}\mathbf{A}^2(0)\,. \qquad (2.175)$$

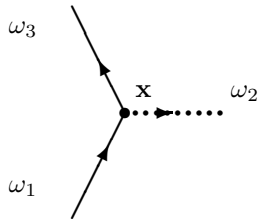
The normal ordered form of H_M taken in the interaction representation must be added to the interaction Hamiltonian. It gives the following additional lines and verteces to the Feynman rules (we assume that the Coulomb gauge is used).

1. *Coulomb contribution.* An additional line ("Coulomb-recoil" line) appears to be



$\frac{i}{2\pi}\frac{\delta_{kl}}{M}\int_{-\infty}^{\infty}d\omega\,.$

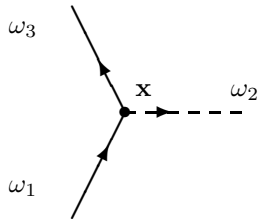
This line joins two vertices each of which corresponds to



$$-2\pi i\gamma^0\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{x}\,p_k\ ,$$

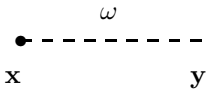
where $\mathbf{p}=-i\nabla_\mathbf{x}$ and $k=1,2,3$.

2. *One-transverse-photon contribution.* An additional vertex on an electron line appears to be



$$-2\pi i\gamma^0\delta(\omega_1-\omega_2-\omega_3)\tfrac{eZ}{M}\int d\mathbf{x}\,p_k\ ,$$

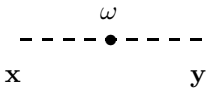
The transverse photon line attached to this vertex (at the point $\mathbf{x}$) is



$\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega D_{kl}(\omega,\mathbf{y})\,.$

At the point $\mathbf{y}$ this line is to be attached to an usual vertex in which we have $-2\pi ie\gamma^0\alpha_l 2\pi\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{y}$, where α_l $(l=1,2,3)$ are the usual Dirac matrices.

3. *Two-transverse-photon contribution.* An additional line ("two-transverse-photon-recoil" line) appears to be



$\frac{i}{2\pi}\frac{e^2Z^2}{M}\int_{-\infty}^{\infty}d\omega D_{il}(\omega,\mathbf{x})D_{lk}(\omega,\mathbf{y})\,.$

This line joins usual vertices (see the previous item).

Let as apply this formalism to the case of a single level a in a one-electron atom. To find the Coulomb nuclear recoil correction we have to calculate the contribution of the diagram shown in Fig. 23. According to the Feynman rules given above we obtain

$$\Delta g^{(1)}_{aa}(E) = \frac{1}{(E-E^{(0)}_a)^2}\frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle a|p_i|n\rangle\langle n|p_i|a\rangle}{\omega-\varepsilon_n(1-i0)}\,. \tag{2.176}$$

The formula (2.51) gives

$$\Delta E_{\rm C} = \frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle a|p_i|n\rangle\langle n|p_i|a\rangle}{\omega-\varepsilon_n(1-i0)}\,. \tag{2.177}$$

The one-transverse-photon nuclear recoil correction corresponds to the diagrams shown in Fig. 24. A similar calculation yields

$$\Delta E_{\rm tr(1)} = \frac{4\pi\alpha Z}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \left\{ \frac{\langle a|p_i|n\rangle\langle n|\alpha_k D_{ik}(\varepsilon_a-\omega)|a\rangle}{\omega-\varepsilon_n(1-i0)} + \frac{\langle a|\alpha_k D_{ik}(\varepsilon_a-\omega)|n\rangle\langle n|p_i|a\rangle}{\omega-\varepsilon_n(1-i0)} \right\}. \tag{2.178}$$

The two-transverse-photon nuclear recoil correction is defined by the diagram shown in Fig. 25. We find

$$\Delta E_{\rm tr(2)} = \frac{(4\pi\alpha Z)^2}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \times\frac{\langle a|\alpha_i D_{il}(\varepsilon_a-\omega)|n\rangle\langle n|\alpha_k D_{lk}(\varepsilon_a-\omega)|a\rangle}{\omega-\varepsilon_n(1-i0)}\,. \tag{2.179}$$

The sum of all the contributions is

$$\Delta E = \frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\, \langle a|(p_i + 4\pi\alpha Z\alpha_l D_{li}(\omega)) \times G_{\rm C}(\omega+\varepsilon_a)(p_i + 4\pi\alpha Z\alpha_m D_{mi}(\omega))|a\rangle\,, \tag{2.180}$$

where $G_{\rm C}(\omega)$ is the Coulomb-Green function defined above. For the practical calculations it is convenient to represent the expression (2.180) as the sum of a low-order term $\Delta E_{\rm L}$ and a higher-order term $\Delta E_{\rm H}$:

$$\Delta E = \Delta E_{\rm L} + \Delta E_{\rm H}\,, \tag{2.181}$$

$$\Delta E_{\rm L} = \frac{1}{2M}\langle a|[p_i^2 - (D_i(0)p_i + p_i D_i(0))]|a\rangle\,, \tag{2.182}$$

$$\Delta E_{\rm H} = \frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\langle a|\Big(D_i(\omega) - \frac{[p_i,V_{\rm C}]}{\omega+i0}\Big)G_{\rm C}(\omega+\varepsilon_a)\Big(D_i(\omega)+\frac{[p_i,V_{\rm C}]}{\omega+i0}\Big)|a\rangle\,, \tag{2.183}$$

where $D_i(\omega) = -4\pi\alpha Z\alpha_l D_{li}(\omega)$. The term $\Delta E_{\rm L}$ contains all the recoil corrections within the $(\alpha Z)^4 m^2/M$ approximation while the term $\Delta E_{\rm H}$ contains the contribution of order $(\alpha Z)^5 m^2/M$ and all contributions of higher orders in αZ which are not included in $\Delta E_{\rm L}$. The formulas (2.181)-(2.183) were first derived by a quasipotential method in Ref. [46] and subsequently rederived by other methods in Refs. [69,70]. The representation (2.180) was found in Ref. [69].

Consider now a two-electron atom. For simplicity, as usual, we assume that the unperturbed wave function is a one-determinant function (2.120). The nuclear recoil correction is the sum of the one-electron and two-electron contributions. Using the Feynman rules and the formula (2.51) one easily finds that the one-electron contribution is equal to the sum of the expressions (2.180) for the a and b states. The two-electron contributions correspond to the diagrams shown in Figs. 26-28. A simple calculation of these diagrams yields

$$\Delta E^{(\rm int)} = \frac{1}{M}\sum_P (-1)^P \langle Pa|p_i + 4\pi\alpha Z\alpha_l D_{li}(\varepsilon_{Pa}-\varepsilon_a)|a\rangle \times\langle Pb|p_i + 4\pi\alpha Z\alpha_m D_{mi}(\varepsilon_{Pb}-\varepsilon_b)|b\rangle\,. \tag{2.184}$$

The formula (2.184) was first derived by a quasipotential method in Ref. [47].

III. TRANSITION PROBABILITIES AND CROSS SECTIONS OF SCATTERING PROCESSES

According to the basic principles of the quantum field theory [71] the number of the particles scattered on the interval $d\mathbf{p}'_1 \cdots d\mathbf{p}'_r$ for a unit time and in a unit volume is

$$dW_{p\to p'} = (2\pi)^{3s+1} n_1 \cdots n_s |\tau_{p'p}|^2 \delta(E_p - E_{p'}) d\mathbf{p}'_1 \cdots d\mathbf{p}'_r \,, \tag{3.1}$$

where p, p' are the initial and final states of the system, respectively; $\tau_{p'p}$ is the amplitude of the process defined by

$$\langle p'|(S-I)|p\rangle = 2\pi i\, \delta(E_p - E_{p'})\tau_{p'p} \,, \tag{3.2}$$

S is the scattering operator, s is the number of the initial particles, r is the number of the final particles; $n_1, ...n_s$ are the average numbers of the particles in the unit volume.

We will consider the scattering of photons and electrons on the atom which is put at the origin of the coordinate system. The differential cross-section is defined by

$$d\sigma = \frac{dW_{p\to p'}}{j} \,, \tag{3.3}$$

where j is the current of the initial particles (for photons $j = nc$; for electrons j=nv, where v is the velocity of the electrons in the nucleus frame). The total cross section can be found by integrating the differential cross section over all final states. The cross section of the elastic scattering is

$$\sigma_{\rm tot}^{\rm (elast)}(p) = \frac{(2\pi)^4}{v} \int d\mathbf{p}' \delta(E_p - E_{p'}) |\tau_{p'p}|^2 \,. \tag{3.4}$$

The total (elastic plus inelastic) cross section can be found by using the optical theorem

$$\sigma_{\rm tot}(p) = \frac{2(2\pi)^3}{v} {\rm Im}\tau_{pp} \,. \tag{3.5}$$

In terms of the amplitude $f_{p'p}$ which is defined so that $d\sigma = |f_{p'p}|^2 d\Omega$, the optical theorem has a well known form (see, e.g., [72])

$$\sigma_{\rm tot}(p) = \frac{4\pi}{|\mathbf{p}|} {\rm Im} f_{pp} \,. \tag{3.6}$$

The aim of this section is to derive formulas for calculation of transition and scattering amplitudes for various processes in the framework of QED.

A. Photon emission by an atom

Consider the process of photon emission by an atom. According to the standard reduction technique (see, e.g., [24,52]), the atomic transition amplitude from state a to state b accompanied with photon emission with momentum $\mathbf{k}_f$ and polarization $\boldsymbol{\epsilon}_f$ is

$$S_{\gamma_f,b;a} = \langle b|a_{\rm out}(k_f,\epsilon_f)|a\rangle = -iZ_3^{-\frac{1}{2}} \int d^4y \frac{\epsilon_f^{\nu *} \exp(ik_f\cdot y)}{\sqrt{2k_f^0(2\pi)^3}} \langle b|j_\nu(y)|a\rangle \,. \tag{3.7}$$

Here $j_\nu(y)$ is the electron-positron current operator in the Heisenberg representation, $|a\rangle$ and $|b\rangle$ are the vectors of the initial and final states in the Heisenberg representation, Z_3 is a renormalization constant, $a\cdot b \equiv a_\nu b^\nu$, $\epsilon_f = (0, \boldsymbol{\epsilon}_f)$, $k_f = (k_f^0, \mathbf{k}_f)$, and $k_f^0 \equiv |\mathbf{k}_f|$. Using the equation (see Appendix A)

$$j^\nu(y) = \exp(iHy^0) j^\nu(0,\mathbf{y}) \exp(-iHy^0) \tag{3.8}$$

one obtains

$$S_{\gamma_f,b;a} = -iZ_3^{-\frac{1}{2}} \int d^4y \exp\left[i(E_b + k_f^0 - E_a)y^0\right] A_f^{\nu *}(\mathbf{y}) \langle b|j_\nu(0,\mathbf{y})|a\rangle$$
$$= -2\pi i Z_3^{-\frac{1}{2}} \delta(E_b + k_f^0 - E_a) \int d\mathbf{y} A_f^{\nu *}(\mathbf{y}) \langle b|j_\nu(0,\mathbf{y})|a\rangle \,, \tag{3.9}$$

where

$$A_f^\nu(\mathbf{x}) = \frac{\epsilon_f^\nu \exp\left(i\mathbf{k}_f \cdot \mathbf{x}\right)}{\sqrt{2k_f^0(2\pi)^3}} \tag{3.10}$$

is the wave function of the emitted photon. Since $|a\rangle$ and $|b\rangle$ are bound states, equation (3.9) as well as the standard reduction technique [24,52] cannot be used for a direct evaluation of the amplitude. A desired calculation formula can be derived within the two-time Green function formalism [26–28].

To formulate the method for a general case, we will assume that in the zeroth approximation the state a belongs to a s_a-dimensional subspace of unperturbed degenerate states Ω_a and the state b belongs to a s_b-dimensional subspace of unperturbed degenerate states Ω_b. The projectors on these subspaces we denote by $P_a^{(0)}$ and $P_b^{(0)}$, respectively. We denote the states coming from Ω_a by $|n_a\rangle$ and the states coming from Ω_b by $|n_b\rangle$. We will also assume that on an intermediate stage of the calculations a non-zero photon mass μ is introduced. It is considered to be larger than the energy splitting of the initial and final states under consideration and much smaller than the distance to other levels.

We introduce in the Heisenberg representation

$$\mathcal{G}_{\gamma_f}(E', E; \mathbf{x}'_1, ...\mathbf{x}'_N; \mathbf{x}_1, ...\mathbf{x}_N)\delta(E' + k^0 - E)$$
$$= \frac{1}{2\pi i}\frac{1}{2\pi}\frac{1}{N!}\int_{-\infty}^{\infty} dx^0 dx'^0 \int d^4y \exp\left(iE'x'^0 - iEx^0\right)\exp\left(ik^0y^0\right)$$
$$\times A_f^{\nu *}(\mathbf{y})\langle 0|T\psi(x'^0, \mathbf{x}'_1)\cdots\psi(x'^0, \mathbf{x}'_N)$$
$$\times j_\nu(y)\overline{\psi}(x^0, \mathbf{x}_N)\cdots\overline{\psi}(x^0, \mathbf{x}_1)|0\rangle \,. \tag{3.11}$$

We will be interested in singularities of $\mathcal{G}_{\gamma_f}$ in vicinity of the points $E' \approx E_b^{(0)}$ and $E \approx E_a^{(0)}$. Using the transformation rules

$$\psi(x^0, \mathbf{x}) = \exp\left(iHy^0\right)\psi(x^0 - y^0, \mathbf{x})\exp\left(-iHy^0\right),$$
$$j(y^0, \mathbf{y}) = \exp\left(iHy^0\right)j(0, \mathbf{y})\exp\left(-iHy^0\right), \tag{3.12}$$

we obtain

$$\mathcal{G}_{\gamma_f}(E', E; \mathbf{x}'_1, ...\mathbf{x}'_N; \mathbf{x}_1, ...\mathbf{x}_N)\delta(E' + k^0 - E)$$
$$= \frac{1}{2\pi i}\frac{1}{2\pi}\frac{1}{N!}\int_{-\infty}^{\infty} dtdt' \int d^4y \exp\left(iE't' - iEt\right)\exp\left[i(E' + k^0 - E)y^0\right]$$
$$\times A_f^{\nu *}(\mathbf{y})\langle 0|T\psi(t', \mathbf{x}'_1)\cdots\psi(t', \mathbf{x}'_N)$$
$$\times j_\nu(0, \mathbf{y})\overline{\psi}(t, \mathbf{x}_N)\cdots\overline{\psi}(t, \mathbf{x}_1)|0\rangle$$
$$= \frac{1}{2\pi i}\delta(E' + k^0 - E)\frac{1}{N!}\int_{-\infty}^{\infty} dtdt' \int d\mathbf{y} \exp\left(iE't' - iEt\right)$$
$$\times A_f^{\nu *}(\mathbf{y})\langle 0|T\psi(t', \mathbf{x}'_1)\cdots\psi(t', \mathbf{x}'_N)$$
$$\times j_\nu(0, \mathbf{y})\overline{\psi}(t, \mathbf{x}_N)\cdots\overline{\psi}(t, \mathbf{x}_1)|0\rangle \,. \tag{3.13}$$

Using again the time-shift transformation rules and denoting, as in the previous section (see equations (2.21) -(2.24)), $E_n \equiv E_n - E_0$ we have

$$\mathcal{G}_{\gamma_f}(E', E; \mathbf{x}'_1, ...\mathbf{x}'_N; \mathbf{x}_1, ...\mathbf{x}_N)$$
$$= \frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty} dtdt' \int d\mathbf{y} \exp\left(iE't' - iEt\right)\sum_{n_1,n_2} A_f^{\nu *}(\mathbf{y})$$
$$\times \exp\left(-iE_{n_1}t'\right)\exp\left(iE_{n_2}t\right)\theta(t')\theta(-t)\langle 0|T\psi(0, \mathbf{x}'_1)\cdots\psi(0, \mathbf{x}'_N)|n_1\rangle$$
$$\times \langle n_1|j_\nu(0, \mathbf{y})|n_2\rangle\langle n_2|\overline{\psi}(0, \mathbf{x}_N)\cdots\overline{\psi}(0, \mathbf{x}_1)|0\rangle + \cdots. \tag{3.14}$$

Taking into account the identities

$$\int_0^\infty dt \exp\left[i(E' - E_{n_1})t\right] = \frac{i}{E' - E_{n_1} + i0}\,,$$
$$\int_{-\infty}^0 dt \exp\left[i(-E + E_{n_2})t\right] = \frac{i}{E - E_{n_2} + i0}\,, \tag{3.15}$$

we find

$$\begin{aligned}
&\mathcal{G}_{\gamma_f}(E', E; \mathbf{x}'_1, ...\mathbf{x}'_N; \mathbf{x}_1, ...\mathbf{x}_N) \\
&= \frac{i}{2\pi}\frac{1}{N!}\sum_{n_1,n_2}\int d\mathbf{y} A_f^{\nu *}(\mathbf{y})\frac{1}{E' - E_{n_1} + i0}\frac{1}{E - E_{n_2} + i0} \\
&\quad \times \langle 0|T\psi(0,\mathbf{x}'_1)\cdots\psi(0,\mathbf{x}'_N)|n_1\rangle\langle n_1|j_\nu(0,\mathbf{y})|n_2\rangle \\
&\quad \times \langle n_2|\overline{\psi}(0,\mathbf{x}_N)\cdots\overline{\psi}(0,\mathbf{x}_1)|0\rangle + \cdots .
\end{aligned} \tag{3.16}$$

We are interested in the analytical properties of $\mathcal{G}_{\gamma_f}$ as a function of two complex variables E' and E in the region $E' \approx E_b^{(0)}$, $E \approx E_a^{(0)}$. These properties can be studied using the complete spectral representation of this type Green function which is given in Appendix E (a similar representation was derived in Ref. [58]). As it follows from the spectral representation, the terms which are omitted in equation (3.16) are regular functions of E' or E when $E' \approx E_b^{(0)}$ and $E \approx E_a^{(0)}$. The equation (3.16) and the spectral representation given in Appendix E show that, for a non-zero photon mass μ, the Green function $\mathcal{G}_{\gamma_f}(E', E)$ has isolated poles in variables E' and E at the points $E' = E_{n_b}$ and $E = E_{n_a}$, respectively. Let us now introduce a Green function $g_{\gamma_f,b;a}(E', E)$ by

$$g_{\gamma_f,b;a}(E', E) = P_b^{(0)}\mathcal{G}_{\gamma_f}(E', E)\gamma_1^0\cdots\gamma_N^0 P_a^{(0)}\,, \tag{3.17}$$

where, as in (2.39), the integration over the electron coordinates is implicit. According to equation (3.16) (see also Appendix E) the Green function $g_{\gamma_f,b;a}(E', E)$ can be written as

$$\begin{aligned}
g_{\gamma_f,b;a}(E', E) = \frac{i}{2\pi}\sum_{n_a=1}^{s_a}\sum_{n_b=1}^{s_b}\frac{1}{E' - E_{n_b}}\frac{1}{E - E_{n_a}}\varphi_{n_b}\int d\mathbf{y} A_f^{\nu *}(\mathbf{y})\langle n_b|j_\nu(0,\mathbf{y})|n_a\rangle\varphi_{n_a}^\dagger \\
+ \text{ terms that are regular functions of } E' \text{ or } E \text{ when } E' \approx E_b^{(0)} \\
\text{and } E \approx E_a^{(0)}\,,
\end{aligned} \tag{3.18}$$

where φ_k are defined by equation (2.65). Let the contours Γ_a and Γ_b surround the poles corresponding to the considered initial and final levels, respectively, and keep outside other singularities of $g_{\gamma_f,b;a}(E', E)$ including the cuts starting from the lower-lying bound states. Comparing equation (3.18) with equation (3.9) and taking into account the biorthogonality condition (2.71) we obtain the desirable formula [26]

$$S_{\gamma_f,b;a} = Z_3^{-1/2}\delta(E_b + k_f^0 - E_a)\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE v_b^\dagger g_{\gamma_f,b;a}(E', E)v_a\,, \tag{3.19}$$

where we imply by a one of the initial states and by b one of the final states under consideration. The vectors v_k are determined from equations (2.76)- (2.77).

In the case of a single initial state (a) and a single final state (b) the vectors v_a and v_b become simply normalization factors. So, for the initial state,

$$v_a^* P_a v_a = v_a^*\frac{1}{2\pi i}\oint_{\Gamma_a} dE g_{aa}(E)v_a = 1 \tag{3.20}$$

and, therefore,

$$|v_a|^2 = \Big[\frac{1}{2\pi i}\oint_{\Gamma_a} dE g_{aa}(E)\Big]^{-1}\,. \tag{3.21}$$

Choosing

$$v_a = \Big[\frac{1}{2\pi i}\oint_{\Gamma_a} dE g_{aa}(E)\Big]^{-1/2}, \qquad v_b = \Big[\frac{1}{2\pi i}\oint_{\Gamma_b} dE g_{bb}(E)\Big]^{-1/2}, \tag{3.22}$$

we find

$$\begin{aligned} S_{\gamma_f,b;a} = Z_3^{-1/2}\delta(E_b + k_f^0 - E_a)\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE g_{\gamma_f,b;a}(E',E) \\ \times\Big[\frac{1}{2\pi i}\oint_{\Gamma_b} dE g_{bb}(E)\Big]^{-1/2}\Big[\frac{1}{2\pi i}\oint_{\Gamma_a} dE g_{aa}(E)\Big]^{-1/2}. \end{aligned} \tag{3.23}$$

For practical calculations of the transition amplitude it is convenient to express the Green function $g_{\gamma_f,b;a}(E',E)$ in terms of the Fourier transform of a $2N$-time Green function

$$\begin{aligned} g_{\gamma_f,b;a}(E',E)\delta(E'+k^0-E) = \frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0 \\ \times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0) \\ \times P_b^{(0)} G_{\gamma_f}(p_1'^0,\ldots,p_N'^0;k^0;p_1^0,\ldots,p_N^0)\gamma_1^0\ldots\gamma_N^0 P_a^{(0)}, \end{aligned} \tag{3.24}$$

where

$$\begin{aligned} &G_{\gamma_f}((p_1'^0,\mathbf{x}_1'),\ldots,(p_N'^0,\mathbf{x}_N');k^0;(p_1^0,\mathbf{x}_1),\ldots,(p_N^0,\mathbf{x}_N)) \\ &= \frac{2\pi}{i}\frac{1}{(2\pi)^{2N+1}}\int_{-\infty}^{\infty} dx_1^0 ... dx_N^0 dx_1'^0 ... dx_N'^0 \int d^4y \\ &\quad\times\exp\left(ip_1'^0x_1'^0 + ... + ip_N'^0x_N'^0 - ip_1^0x_1^0 - ... - ip_N^0x_N^0 + ik^0y^0\right) \\ &\quad\times A_f^{\nu *}(\mathbf{y})\langle 0|T\psi(x_1')\cdots\psi(x_N')j_\nu(y)\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle . \end{aligned} \tag{3.25}$$

The Green function G_{γ_f} is constructed by perturbation theory after the transition in (3.25) to the interaction representation and using Wick's theorem. The Feynman rules for G_{γ_f} differ from those for G considered in the previous section only by presence of an outgoing photon line which corresponds to the wave function of the emitted photon $A_f^{\nu *}(\mathbf{x})$. The Feynman rule for a vertex in which a real photon is emitted remains the same as for a virtual photon vertex. The energy variable of the emitted photon (k^0) in the expression corresponding to a real photon vertex is considered as a free variable ($k^0 \neq k_f^0 = |\mathbf{k}_f|$) which, due to the energy conservation, can be expressed in terms of the initial (E) and final (E') atomic energy variables.

B. Transition probability in a one-electron atom

To demonstrate the practical ability of the formalism, in this section we derive formulas for the transition probability in a one-electron atom to zeroth and first orders in α. An application of the method for two-electron atoms is considered in [73].

1. Zeroth order approximation

To zeroth order the transition amplitude is described by the diagram shown in Fig. 29. The formula (3.23) gives

$$S_{\gamma_f,b;a}^{(0)} = \delta(E_b + k_f^0 - E_a)\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g_{\gamma_f,b;a}^{(0)}(E',E), \tag{3.26}$$

where the superscript indicates the order in α. Here we have taken into account that

$$\frac{1}{2\pi i}\oint_{\Gamma_a} dE\, g_{aa}^{(0)}(E) = \frac{1}{2\pi i}\oint_{\Gamma_a} dE \frac{1}{E-\varepsilon_a} = 1 \tag{3.27}$$

and a similar equation for the b state. According to the Feynman rules we have

$$G^{(0)}_{\gamma_f}((E,'\mathbf{x}');k^0;(E,\mathbf{x})) = \int d\mathbf{y}\frac{i}{2\pi}S(E',\mathbf{x}',\mathbf{y})(-2\pi ie\gamma^\nu)\delta(E'+k^0-E)$$
$$\times A^*_{f,\nu}(\mathbf{y})\frac{i}{2\pi}S(E,\mathbf{y},\mathbf{x})\,. \tag{3.28}$$

Substituting the expression (3.28) into the definition of $g_{\gamma_f,b;a}(E',E)$ (see equation (3.24)), we obtain

$$g_{\gamma_f,b;a}(E',E) = \frac{i}{2\pi}\frac{1}{E'-\varepsilon_b}\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle\frac{1}{E-\varepsilon_a}\,. \tag{3.29}$$

The equations (3.26), (3.29) yield

$$S^{(0)}_{\gamma_f,b;a} = -2\pi i\,\delta(E_b+k^0_f-E_a)\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle \tag{3.30}$$

or according to the definition (3.2)

$$\tau^{(0)}_{\gamma_f,b;a} = -\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle = \langle b|e\boldsymbol{\alpha}\cdot\mathbf{A}^*_f|a\rangle\,. \tag{3.31}$$

According to equation (3.1), the transition probability to zeroth order is

$$dW^{(0)}_{\gamma_f,b;a} = 2\pi|\tau^{(0)}_{\gamma_f,b;a}|^2\delta(E_b+k^0_f-E_a)d\mathbf{k}_f$$
$$= 2\pi\frac{e^2}{2k^0_f(2\pi)^3}|\langle b|\epsilon^{\nu *}_f\alpha_\nu\exp(-i\mathbf{k}_f\cdot\mathbf{x})|a\rangle|^2\delta(E_b+k^0_f-E_a)d\mathbf{k}_f\,. \tag{3.32}$$

Integrating over the photon energy one finds

$$dW^{(0)}_{\gamma_f,b;a} = \alpha\frac{k^0_f}{2\pi}|\boldsymbol{\epsilon}^*_f\cdot\mathbf{j}_{ba}(\mathbf{k}_f)|^2d\Omega_f\,, \tag{3.33}$$

where

$$\mathbf{j}_{ba}(\mathbf{k}_f) = \langle b|\boldsymbol{\alpha}\exp(-i\mathbf{k}_f\cdot\mathbf{x})|a\rangle\,. \tag{3.34}$$

2. QED corrections of first order in α

The QED corrections of first order in α are defined by the diagrams shown in Fig. 30. Let us consider in detail the derivation of the formulas for the self-energy (SE) corrections (the diagrams (a)-(c)). The formula (3.23) gives in the order under consideration

$$S^{(1)}_{\gamma_f,b;a} = \delta(E_b+k^0_f-E_a)\Big\{\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\,g^{(1)}_{\gamma_f,b;a}(E',E)$$
$$-\frac{1}{2}\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\,g^{(0)}_{\gamma_f,b;a}(E',E)\Big[\frac{1}{2\pi i}\oint_{\Gamma_b}dE\,g^{(1)}_{bb}(E)+\frac{1}{2\pi i}\oint_{\Gamma_a}dE\,g^{(1)}_{aa}(E)\Big]\Big\}\,, \tag{3.35}$$

where $g^{(1)}_{aa}(E)$ and $g^{(1)}_{bb}(E)$ are defined by the first-order self-energy diagram. Here we have omitted a term of first order in α which comes from the factor $Z_3^{-1/2}$ since it has to be combined with the vacuum-polarization (VP) correction. Consider first the diagram (a). According to the Feynman rules, we have

$$G^{(1,a)}_{\gamma_f}((E',\mathbf{x}');k^0;(E,\mathbf{x})) = \delta(E'+k^0-E)\int d\mathbf{y}d\mathbf{y}'d\mathbf{z}\,\frac{i}{2\pi}S(E',\mathbf{x}',\mathbf{y})\frac{2\pi}{i}\gamma^0\Sigma(E',\mathbf{y}',\mathbf{y})$$
$$\times\frac{i}{2\pi}S(E',\mathbf{y},\mathbf{z})A^*_{f,\nu}(\mathbf{z})(-2\pi ie\gamma^\nu)\frac{i}{2\pi}S(E,\mathbf{z},\mathbf{x})\,, \tag{3.36}$$

where

$$\Sigma(E',\mathbf{y}',\mathbf{y}) = e^2\frac{i}{2\pi}\int d\omega\,\gamma^0\gamma^\rho S(E'-\omega,\mathbf{y}',\mathbf{y})\gamma^\sigma D_{\rho\sigma}(\omega,\mathbf{y}'-\mathbf{y}) \tag{3.37}$$

is the kernel of the self-energy operator and $D_{\rho\sigma}(\omega, \mathbf{y}' - \mathbf{y})$ is the photon propagator for a non-zero photon mass. According to the definition of $g_{\gamma_f,b;a}(E', E)$ (see equation (3.24)) one finds

$$g^{(1,a)}_{\gamma_f,b;a}(E', E) = \frac{i}{2\pi} \sum_n \frac{\langle b|\Sigma(E')|n\rangle\langle n|e\alpha^\nu A^*_{f,\nu}|a\rangle}{(E' - \varepsilon_b)(E' - \varepsilon_n)(E - \varepsilon_a)} \tag{3.38}$$

and

$$\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(1,a)}_{\gamma_f,b;a}(E', E) = -2\pi i \Big[\sum_n^{n\neq b} \frac{\langle b|\Sigma(\varepsilon_b)|n\rangle\langle n|e\alpha^\nu A^*_{f,\nu}|a\rangle}{\varepsilon_b - \varepsilon_n} + \langle b|\Sigma'(\varepsilon_b)|b\rangle\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle \Big] , \tag{3.39}$$

where $\Sigma'(\varepsilon_b) \equiv \frac{d\Sigma(\varepsilon)}{d\varepsilon}\Big|_{\varepsilon=\varepsilon_b}$. A similar calculation of the diagram (b) gives

$$\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(1,c)}_{\gamma_f,b;a}(E', E) = -2\pi i \Big[\sum_n^{n\neq a} \frac{\langle b|e\alpha^\nu A^*_{f,\nu}|n\rangle\langle n|\Sigma(\varepsilon_a)|a\rangle}{\varepsilon_a - \varepsilon_n} + \langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle \Big] . \tag{3.40}$$

The second ("reducible") terms in equations (3.39) and (3.40) are to be combined with the second term in equation (3.35). Taking into account that

$$\frac{1}{2\pi i} \oint_{\Gamma_a} dE\, g^{(1)}_{aa}(E) = \langle a|\Sigma'(\varepsilon_a)|a\rangle , \tag{3.41}$$

$$\frac{1}{2\pi i} \oint_{\Gamma_b} dE\, g^{(1)}_{bb}(E) = \langle b|\Sigma'(\varepsilon_b)|b\rangle , \tag{3.42}$$

we obtain

$$-\frac{1}{2} \oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(0)}_{\gamma_f,b;a}(E', E) \Big[\frac{1}{2\pi i} \oint_{\Gamma_b} dE\, g^{(1)}_{bb}(E) + \frac{1}{2\pi i} \oint_{\Gamma_a} dE\, g^{(1)}_{aa}(E) \Big] = 2\pi i \Big[\frac{1}{2} \langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle (\langle b|\Sigma'(\varepsilon_b)|b\rangle + \langle a|\Sigma'(\varepsilon_a)|a\rangle) \Big] . \tag{3.43}$$

For the diagram (c) we find

$$g^{(1,b)}_{\gamma_f,b;a}(E', E) = \frac{i}{2\pi} \frac{1}{E' - \varepsilon_b} \int d\mathbf{x} d\mathbf{y} d\mathbf{z} \overline{\psi}_b(\mathbf{x}) \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \gamma^\rho S(E' - \omega, \mathbf{x}, \mathbf{z}) \times eA^*_\nu(\mathbf{z}) \gamma^\nu S(E - \omega, \mathbf{z}, \mathbf{y}) \gamma^\sigma e^2 D_{\rho\sigma}(\omega, \mathbf{x} - \mathbf{y}) \psi_a(\mathbf{y}) \frac{1}{E - \varepsilon_a} . \tag{3.44}$$

Substituting (3.44) into (3.35) we obtain

$$\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(1,b)}_{\gamma_f,b;a}(E', E) = = -2\pi i \int d\mathbf{z}\, eA^*_{f,\nu}(\mathbf{z}) \Lambda^\nu(\varepsilon_b, \varepsilon_a, \mathbf{z}) , \tag{3.45}$$

where

$$\Lambda^\nu(\varepsilon_b, \varepsilon_a, \mathbf{z}) = e^2 \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \int d\mathbf{x} d\mathbf{y}\, \overline{\psi}_b(\mathbf{x}) \gamma^\rho S(\varepsilon_b - \omega, \mathbf{x}, \mathbf{z}) \gamma^\nu S(\varepsilon_a - \omega, \mathbf{z}, \mathbf{y}) \times \gamma^\sigma D_{\rho\sigma}(\omega, \mathbf{x} - \mathbf{y}) \psi_a(\mathbf{y}) . \tag{3.46}$$

Summing all the first order SE contributions derived above and adding the contribution of the mass counterterm diagrams (Fig. 31), we find

$$S^{(1,\mathrm{SE})}_{\gamma_f,b;a} = -2\pi i\,\delta(E_b + k_f^0 - E_a)\,\Big[\sum_n^{n\neq b}\frac{\langle b|\Sigma(\varepsilon_b) - \beta\delta m|n\rangle\langle n|e\alpha^\nu A^*_{f,\nu}|a\rangle}{\varepsilon_b - \varepsilon_n}$$
$$+\sum_n^{n\neq a}\frac{\langle b|e\alpha^\nu A^*_{f,\nu}|n\rangle\langle n|\Sigma(\varepsilon_a) - \beta\delta m|a\rangle}{\varepsilon_a - \varepsilon_n}$$
$$+\int d\mathbf{z}\, eA^*_{f,\nu}(\mathbf{z})\Lambda^\nu(\varepsilon_b,\varepsilon_a,\mathbf{z})$$
$$+\frac{1}{2}\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle(\langle b|\Sigma'(\varepsilon_b)|b\rangle + \langle a|\Sigma'(\varepsilon_a)|a\rangle)\Big]\,. \tag{3.47}$$

A similar calculation of the vacuum-polarization diagrams (Fig. 30, diagrams (d)-(f)) gives

$$S^{(1,\mathrm{VP})}_{\gamma_f,b;a} = -2\pi i\,\delta(E_b + k_f^0 - E_a)\,\Big[\sum_n^{n\neq b}\frac{\langle b|U_{\mathrm{VP}}|n\rangle\langle n|e\alpha^\nu A^*_{f,\nu}|a\rangle}{\varepsilon_b - \varepsilon_n}$$
$$+\sum_n^{n\neq a}\frac{\langle b|e\alpha^\nu A^*_{f,\nu}|n\rangle\langle n|U_{\mathrm{VP}}|a\rangle}{\varepsilon_a - \varepsilon_n}$$
$$+\int d\mathbf{z}\, eA^*_{f,\nu}(\mathbf{z})Q^\nu(k_f^0,\mathbf{z}) + (Z_3^{-1/2} - 1)\langle b|e\alpha^\nu A^*_{f,\nu}|a\rangle\Big]\,, \tag{3.48}$$

where

$$U_{\mathrm{VP}}(\mathbf{x}) = \frac{\alpha}{2\pi i}\int d\mathbf{y}\,\frac{1}{|\mathbf{x}-\mathbf{y}|}\int_{-\infty}^{\infty} d\omega\,\mathrm{Tr}[S(\omega,\mathbf{y},\mathbf{y})\gamma^0] \tag{3.49}$$

is the VP potential and

$$Q^\nu(k^0,\mathbf{z}) = -e^2\int d\mathbf{x}d\mathbf{y}\,\overline{\psi}_b(\mathbf{x})\gamma^\rho\psi_a(\mathbf{x})D_{\rho\sigma}(k^0,\mathbf{x}-\mathbf{y})$$
$$\times\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\mathrm{Tr}[\gamma^\sigma S(\omega,\mathbf{y},\mathbf{z})\gamma^\nu S(\omega+k^0,\mathbf{z},\mathbf{y})]\,. \tag{3.50}$$

Some individual terms in equations (3.47) and (3.48) contain ultraviolet divergences. These divergences arise solely from the zero- and one-potential terms in the expansion of the electron propagators in powers of the Coulomb potential. Using the standard expressions for the divergent parts of the zero- and one-potential SE terms (see, e.g., [24]) and the Ward identity ($Z_1 = Z_2$) one easily finds that the ultraviolet divergences cancel each other in equation (3.47). As to equation (3.48), the divergent parts incorporate into the charge renormalization factor ($e = Z_3^{1/2}e_0$).

An alternative approach to the renormalization problem consists in using from the very beginning the renormalized field operators $\psi_R = Z_2^{-1/2}\psi$, $A_R = Z_3^{-1/2}A$, the renormalized electron charge $e = e_0 + \delta e = Z_1^{-1}Z_2Z_3^{1/2}e_0$ and, respectively, the renormalized Green functions. In this approach, additional counterterms arise in the Feynman rules.

The vertex and reducible contributions to the SE corrections (third and fourth terms in equation (3.47)) contain infrared divergences which cancel each other when are summed.

In addition to the QED corrections derived in this subsection, we must take into account the contribution originating from changing the photon energy in the zeroth-order transition probability (3.33) due to the QED correction to the energies of the bound states a and b. It follows that the total QED correction of first order in α to the transition probability is given by

$$dW^{(1)}_{\gamma_f,b;a} = 2\pi(k_f^0)^2 2\mathrm{Re}\Big\{\tau^{(0)*}_{\gamma_f,b;a}\tau^{(1)}_{\gamma_f,b;a}\Big\}d\Omega_f + \Big[dW^{(0)}_{\gamma_f,b;a}\Big|_{k_f^0=E_b-E_a} - dW^{(0)}_{\gamma_f,b;a}\Big|_{k_f^0=\varepsilon_b-\varepsilon_a}\Big]\,. \tag{3.51}$$

Here $\tau^{(1)}_{\gamma_f,b;a} = \tau^{(1,\mathrm{SE})}_{\gamma_f,b;a} + \tau^{(1,\mathrm{VP})}_{\gamma_f,b;a}$ is the QED correction given by equations (3.47) and (3.48) in accordance with the definition (3.2). E_a, E_b and ε_a, ε_b are the energies of the bound states a and b with and without the QED correction, respectively.

C. Radiative recombination of an electron with an atom

In calcualtions of processes which contain a free electron in the initial or final (or in both) states we consider that the interaction with the Coulomb field of the nucleus $V_{\rm C}(\mathbf{x})$ is included in the source $\tilde{j}(x)$ which leads to a scattering [52],

$$(i\,\partial\!\!\!/ - m)\psi(x) = \tilde{j}(x)\,. \tag{3.52}$$

It means that, after the transition to the "in" operators, the unperturbed Hamiltonian does not contain the interaction with the Coulomb potential. As a result, the Feynman rules contain free-electron propagators, instead of the bound-electron ones, and the vertices corresponding to the interaction of electrons with $V_{\rm C}(\mathbf{x})$ appear. Since we consider the case of a strong Coulomb field, we will sum up infinite sequences of Feynman diagrams describing the interaction of electrons with the Coulomb potential. As a result of this summation, the free-electron propagators are replaced by the bound-electron propagators,

$$\begin{aligned}[p^0 - H(1-i0)]^{-1} = {}& [p^0 - H_0(1-i0)]^{-1} \\ & + [p^0 - H_0(1-i0)]^{-1} V_{\rm C} [p^0 - H_0(1-i0)]^{-1} + \cdots\,,\end{aligned} \tag{3.53}$$

where $H = H_0 + V_{\rm C}$ and $H_0 = -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta m$, and the free-electron wave functions are replaced by the wave functions in the Coulomb field. For instance, the wave function of an incident electron with momentum $\mathbf{p}_i$ and polarization μ_i is

$$\begin{aligned}\psi_{p_i\mu_i(+)} &= U_{p_i\mu_i} + [p_i^0 - H_0(1-i0)]^{-1} V_{\rm C} U_{p_i\mu_i} \\ &\quad + [p_i^0 - H_0(1-i0)]^{-1} V_{\rm C} [p_i^0 - H_0(1-i0)]^{-1} V_{\rm C} U_{p_i\mu_i} + \cdots \\ &= U_{p_i\mu_i} + [p_i^0 - H(1-i0)]^{-1} V_{\rm C} U_{p_i\mu_i}\,,\end{aligned} \tag{3.54}$$

where $p_i = (p_i^0, \mathbf{p}_i)$, $p_i^0 = \sqrt{\mathbf{p}_i^2 + m^2}$,

$$U_{p_i\mu_i} = \frac{u(p_i,\mu_i)\exp(i\mathbf{p}_i\cdot\mathbf{x})}{\sqrt{(p_i^0/m)(2\pi)^3}} \tag{3.55}$$

is the free wave function of the incident electron, and $u(p_i,\mu_i)$ is normalized by the condition $\overline{u}u = 1$.

Consider the process of the radiative recombination of an electron with momentum $\mathbf{p}_i$ and polarization μ_i with an $(N-1)$-electron atom $X^{(Z-N+1)+}$ in a state a. As a result of the process the N-electron atom $X^{(Z-N)+}$ in a state b and a photon with momentum $\mathbf{k}_f$ and polarization $\epsilon_f = (0, \boldsymbol{\epsilon}_f)$ arise,

$$e^-(p_i,\mu_i) + X^{(Z-N+1)+}(a) \to \gamma(k_f,\epsilon_f) + X^{(Z-N)+}(b)\,, \tag{3.56}$$

where $k_f = (k_f^0, \mathbf{k}_f)$ and $k_f^0 = |\mathbf{k}_f|$. In this section we will assume that we consider a non-resonance process. It means that the total initial energy $(p_i^0 + E_a)$ is not close to any excited state energy of the N-electron atom. As to the resonance recombination, a detailed description of this process is given in [33] (see also the next sections of this paper).

According to the standard reduction technique [24,52] the amplitude of the process is

$$\begin{aligned}S_{\gamma_f,b;e_i,a} &= \langle b|a_{\rm out}(k_f,\epsilon_f) b^\dagger_{\rm in}(p_i,\mu_i)|a\rangle \\ &= (-iZ_3^{-\frac{1}{2}})(-iZ_2^{-\frac{1}{2}}) \int d^4y d^4z \frac{\epsilon_f^{\nu *}\exp(ik_f\cdot y)}{\sqrt{2k_f^0(2\pi)^3}} \\ &\quad \times \langle b|T j_\nu(y)\overline{\psi}(z)|a\rangle (-i\overleftarrow{\partial\!\!\!/}_z - m) \frac{u(p_i,\mu_i)\exp(-ip_i\cdot z)}{\sqrt{\frac{p_i^0}{m}(2\pi)^3}}\,,\end{aligned} \tag{3.57}$$

where $|a\rangle, |b\rangle$ are the vectors of the initial and final states in the Heisenberg representation. Taking into account that

$$\overline{\psi}(z)(-i\overleftarrow{\partial\!\!\!/}_z - m) = e\overline{\psi}(z)A(z) \equiv \overline{\eta}(z) \tag{3.58}$$

one obtains

$$S_{\gamma_f,b;e_i,a} = 2\pi\delta(E_b + k_f^0 - E_a - p_i^0)(-iZ_3^{-\frac{1}{2}})(-iZ_2^{-\frac{1}{2}}) \int d\mathbf{y}d\mathbf{z} A_f^{\nu *}(\mathbf{y})$$
$$\times\{\int_0^\infty d\tau\ \langle b|j_\nu(\tau,\mathbf{y})\overline{\eta}(0,\mathbf{z})|a\rangle \exp(ik_f^0\tau)$$
$$+\int_0^\infty d\tau\ \langle b|\overline{\eta}(\tau,\mathbf{z})j_\nu(0,\mathbf{y})|a\rangle \exp(-ip_i^0\tau)$$
$$-i\langle b|[\psi^\dagger(0,\mathbf{z}),\ j_\nu(0,\mathbf{y})]|a\rangle\} U_{p_i\mu_i}(\mathbf{z})\,, \tag{3.59}$$

where $A_f^\nu(\mathbf{y})$ is the wave function of the emitted photon defined by equation (3.10) and $U_{p_i\mu_i}(\mathbf{z})$ is the free wave function of the incident electron defined by equation (3.55). To construct the perturbation theory for the amplitude of the process we introduce the Fourier transform of the corresponding two-time Green function

$$\mathcal{G}_{\gamma_f;e_i}(E',E,p^0;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_{N-1})\delta(E'+k^0-E-p^0)$$
$$= \Big(\frac{i}{2\pi}\Big)^2 \frac{1}{\sqrt{N!}}\frac{1}{\sqrt{(N-1)!}}\int_{-\infty}^\infty dx^0dx'^0\ \exp(iE'x'^0 - iEx^0)$$
$$\times\int d^4yd^4z \exp(ik^0y^0 - ip^0z^0)A_f^{\nu *}(\mathbf{y})$$
$$\times\langle 0|T\psi(x'^0,\mathbf{x}'^0_1)\cdots\psi(x'^0,\mathbf{x}'_N)j_\nu(y)\overline{\psi}(z)\overline{\psi}(x^0,\mathbf{x}_{N-1})\cdots\overline{\psi}(x^0,\mathbf{x}_1)|0\rangle$$
$$\times(-i\overleftarrow{\not\partial}_z - m)U_{p_i\mu_i}(\mathbf{z})\,. \tag{3.60}$$

As in the derivation of the formulas for the transition amplitudes, we will assume that in zeroth approximation the initial and final states are degenerate in energy with some other states and will use the same notations for these states as in section III A. As usual, we also assume that a non-zero photon mass μ is introduced. The spectral representation of $\mathcal{G}_{\gamma_f;e_i}(E',E,p^0)$, which can be derived in the same way as for the Green function describing the transition amplitude (see section IIIA and Appendix E), gives

$$\mathcal{G}_{\gamma_f;e_i}(E',E,p^0;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_{N-1})$$
$$= \frac{1}{2\pi}\frac{1}{\sqrt{N!}}\frac{1}{\sqrt{(N-1)!}}\sum_{n_a=1}^{s_a}\sum_{n_b=1}^{s_b}\frac{1}{E'-E_{n_b}}\frac{1}{E-E_{n_a}}$$
$$\times\int d\mathbf{y}d\mathbf{z}\ A_f^{\nu *}(\mathbf{y})\langle 0|T\psi(0,\mathbf{x}'^0_1)\cdots\psi(0,\mathbf{x}'_N)|n_b\rangle$$
$$\times\{\int_0^\infty d\tau\ \langle n_b|j_\nu(\tau,\mathbf{y})\overline{\eta}(0,\mathbf{z})|n_a\rangle \exp(i(E-E_{n_b}+p^0)\tau)$$
$$+\int_0^\infty d\tau\ \langle n_b|\overline{\eta}(\tau,\mathbf{z})j_\nu(0,\mathbf{y})|n_a\rangle \exp(i(E'-E_{n_b}-p^0)\tau)$$
$$-i\langle n_b|[\psi^\dagger(0,\mathbf{z}),\ j_\nu(0,\mathbf{y})]|n_a\rangle\}\langle n_a|\overline{\psi}(0,\mathbf{x}_{N-1})\cdots\overline{\psi}(0,\mathbf{x}_1)|0\rangle U_{p_i\mu_i}(\mathbf{z})$$
$$+ \text{ terms that are regular functions of } E' \text{ or } E \text{ when } E'\approx E_b^{(0)}$$
$$\text{and } E\approx E_a^{(0)}\,. \tag{3.61}$$

We introduce the Green function $g(E',E,p^0)$ by

$$g_{\gamma_f,b;e_i,a}(E',E,p^0) = P_b^{(0)}\mathcal{G}_{\gamma_f;e_i}(E',E,p^0)\gamma_1^0\cdots\gamma_{N-1}^0P_a^{(0)}\,. \tag{3.62}$$

From equation (3.61) we have

$$g_{\gamma_f,b;e_i,a}(E',E,p^0) = \frac{1}{2\pi}\sum_{n_a=1}^{s_a}\sum_{n_b=1}^{s_b}\frac{\varphi_{n_b}}{E'-E_{n_b}}\int d\mathbf{y}d\mathbf{z}\ A_f^{\nu *}(\mathbf{y})$$
$$\times\{\int_0^\infty d\tau\ \langle n_b|j_\nu(\tau,\mathbf{y})\overline{\eta}(0,\mathbf{z})|n_a\rangle \exp(i(E-E_{n_b}+p^0)\tau)$$
$$+\int_0^\infty d\tau\ \langle n_b|\overline{\eta}(\tau,\mathbf{z})j_\nu(0,\mathbf{y})|n_a\rangle \exp(i(E'-E_{n_a}-p^0)\tau)$$

$$-i\langle n_b|[\psi^\dagger(0,\mathbf{z}),\, j_\nu(0,\mathbf{y})]|n_a\rangle\}U_{p_i\mu_i}(\mathbf{z})\frac{\varphi^\dagger_{n_a}}{E-E_{n_a}}$$

$$+ \text{ terms that are regular functions of } E' \text{ or } E \text{ when } E'\approx E_b^{(0)} \text{ and } E\approx E_a^{(0)}\,, \tag{3.63}$$

where φ_{n_a} and φ_{n_b} are the wave functions of the initial and final states defined above. Let the contours Γ_a and Γ_b surround the poles corresponding to the initial and final levels, respectively, and keep outside other singularities of $g_{\gamma_f,b;e_i,a}(E',E,p^0)$. It can be done if the photon mass μ is chosen as indicated in section III A. Taking into account the biorthogonality condition (2.71) and comparing (3.63) with (3.59) we get the desirable formula [33]

$$S_{\gamma_f,b;e_i,a}=(Z_2Z_3)^{-\frac{1}{2}}\delta(E_b+k_f^0-E_a-p_i^0)\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\; v_b^\dagger g_{\gamma_f,b;e_i,a}(E',E,p_i^0)v_a\,, \tag{3.64}$$

where we imply by a one of the initial states and by b one of the final states under consideration. In the case of a single initial state (a) and a single final state (b) it yields

$$S_{\gamma_f,b;e_i,a}=(Z_2Z_3)^{-\frac{1}{2}}\delta(E_b+k_f^0-E_a-p_i^0)\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE g_{\gamma_f,b;e_i,a}(E',E,p_i^0)$$
$$\times\Big[\frac{1}{2\pi i}\oint_{\Gamma_b}dE g_{bb}(E)\Big]^{-1/2}\Big[\frac{1}{2\pi i}\oint_{\Gamma_a}dE g_{aa}(E)\Big]^{-1/2}\,. \tag{3.65}$$

For practical calculations by perturbation theory it is convenient to express the Green function $g_{\gamma_f,b;e_i,a}$ in terms of the Fourier transform of the $(2N-1)$-time Green function

$$g_{\gamma_f,b;e_i,a}(E',E,p^0)\delta(E'+k^0-E-p^0)$$
$$=\frac{1}{\sqrt{N!(N-1)!}}\int_{-\infty}^{\infty}dp_1^0\cdots dp_{N-1}^0dp_1'^0\cdots dp_N'^0\;\delta(E-p_1^0\cdots-p_{N-1}^0)\delta(E'-p_1'^0\cdots-p_N'^0)$$
$$\times P_b^{(0)}G_{\gamma_f;e_i}(p_1'^0,...,p_N'^0;k^0,p^0;p_1^0,...,p_{N-1}^0)\gamma_1^0\cdots\gamma_{N-1}^0P_a^{(0)}\,, \tag{3.66}$$

where

$$G_{\gamma_f;e_i}((p_1'^0,\mathbf{x}_1'),...,(p_N'^0,\mathbf{x}_N');k^0,p^0;(p_1^0,\mathbf{x}_1),...,(p_{N-1}^0,\mathbf{x}_{N-1}))$$
$$=\Big(\frac{2\pi}{i}\Big)^2\frac{1}{(2\pi)^{2N+1}}\int_{-\infty}^{\infty}dx_1^0\cdots dx_{N-1}^0dx_1'^0\cdots dx_N'^0$$
$$\times\exp\left(ip_1'^0x_1'^0+\cdots+ip_N'^0x_N'^0-ip_1^0x_1^0-\cdots-ip_{N-1}^0x_{N-1}^0\right)$$
$$\times\int d^4yd^4z\exp\left(ik^0y^0-ip^0z^0\right)A_f^{\nu*}(\mathbf{y})$$
$$\times\langle 0|T\psi(x_1')\cdots\psi(x_N')j_\nu(y)\overline{\psi}(z)\overline{\psi}(x_{N-1})\cdots\overline{\psi}(x_1)|0\rangle$$
$$\times(-i\overleftarrow{\partial}_z-m)U_{p_i\mu_i}(\mathbf{z})\,. \tag{3.67}$$

The Green function G_{γ_f,e_i} is constructed using Wick's theorem after the transition in (3.67) to the interaction representation. Since we have not included the interaction with $V_{\rm C}$ in the unperturbed Hamiltonian, the Feynman rules contain the free electron propagators and the verteces corresponding to the interaction with $V_{\rm C}$. Summing over all the insertions of the verteces with $V_{\rm C}$ in the electron lines we replace the free electron propagators and wave functions by the electron propagators and wave functions in the Coulomb field according to equations (3.53) (3.54). The free wave function of the incident electron $U_{p_i\mu_i}(\mathbf{x})$ is replaced by the wave function $\psi_{p_i\mu_i(+)}(\mathbf{x})$ which can be determined from the equation

$$\psi_{p_i,\mu_i(+)}=U_{p_i\mu_i}+(p_i^0-H_0(1-i0))^{-1}V_{\rm C}\psi_{p_i\mu_i(+)}\,. \tag{3.68}$$

The wave function $\psi_{p_i\mu_i(+)}(\mathbf{x})$ is a solution of the Dirac equation with the Coulomb potential $V_{\rm C}(\mathbf{x})$ which satisfies the boundary condition [74]

$$\psi_{p\mu(+)}(\mathbf{x})\;\sim\;U_{p\mu}(\mathbf{x})+G^+(\hat{\mathbf{n}})\frac{\exp\left(i|\mathbf{p}||\mathbf{x}|\right)}{|\mathbf{x}|}\,,\qquad|\mathbf{x}|\to\infty\,, \tag{3.69}$$

where $G^+(\hat{\mathbf{n}})$ is a bispinor depending on $\hat{\mathbf{n}} \equiv \mathbf{x}/|\mathbf{x}|$. The apparent expressions for $\psi_{p\mu(+)}(\mathbf{x})$ are given in [74]. Thus, we again revert to the Furry picture. The Feynman rules for $G_{\gamma_f;e_i}$ differ from those for G_{γ_f} only by a replacement of one of the incoming electron propagators $\frac{i}{2\pi}S(\omega,\mathbf{x},\mathbf{y})$ by the wave function $\psi_{p_i\mu_i(+)}(\mathbf{x})$.

In calculations by perturbation theory a problem appears which is caused by the fact that in zeroth approximation the energy of the $N-1$-electron atom may coincide with the difference of the N-electron energy and the one-electron energy. As a result, some of the terms which are omitted in equation (3.61) are singular functions of E' and E when $E' \approx E_b^{(0)}$ and $E \approx E_a^{(0)}$. A special analysis of the complete spectral representation of the Green function $\mathcal{G}_{\gamma_f,e_i}$ shows that to eliminate these terms in calculations by formula (3.64) one may use the following prescription: integrate first over E and keep the point $E = E_a^{(0)} + (E' - E_b^{(0)})$ outside the contour Γ_a.

In Refs. [41,42] this method was used to derive formulas for the QED corrections to the radiative recombination of an electron with a bare nucleus and for the interelectronic-interaction corrections to the radiative recombination of an electron with a high-Z heliumlike atom. Below we consider another application of the method.

D. Radiative recombination of an electron with a high-Z hydrogenlike atom

As a practical application of the method, in this section we derive formulas for the radiative recombination of an electron with a high-Z hydrogenlike ion to zeroth and first orders in $1/Z$. We will assume that the final state of the heliumlike ion is described by a one-determinant wave function

$$u_b(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\sum_P (-1)^P \psi_{Pb_1}(\mathbf{x}_1)\psi_{Pb_2}(\mathbf{x}_2) \tag{3.70}$$

and the one-electron state $|b_1\rangle$ coincides with the initial state $|a\rangle$ of the hydrogenlike ion.

1. Zeroth order approximation

To the zeroth order the radiative recombination amplitude is described by the diagram shown in Fig. 32. The formula (3.65) gives

$$S^{(0)}_{\gamma_f,b;e_i,a} = \delta(E_b + k_f^0 - E_a - p_i^0)\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\,, \tag{3.71}$$

where the superscript indicates the order in α. According to the definition (3.66) and the Feynman rules we have

$$\begin{aligned}
&g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\delta(E'+k^0-E-p_i^0)\\
&= \frac{i}{2\pi}\sum_P (-1)^P \int_{-\infty}^{\infty} dp_1'^0 dp_2'^0 \delta(E'-p_1'^0-p_2'^0)\frac{1}{p_2'^0-\varepsilon_{Pb_2}+i0}\\
&\times\langle Pb_2|e\alpha_\nu A_f^{\nu *}|p\rangle\delta(p_2'^0+k^0-p_i^0)\frac{1}{p_1'^0-\varepsilon_a+i0}\delta(p_1'^0-E)\langle Pb_1|a\rangle\,,
\end{aligned} \tag{3.72}$$

where $|p\rangle \equiv |p_i,\mu_i\rangle$ denotes the state vector of the incident electron. One obtains

$$g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0) = \frac{i}{2\pi}\frac{1}{E'-E-\varepsilon_{b_2}}\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle\frac{1}{E-\varepsilon_a}\,. \tag{3.73}$$

Following to the rule for the integration over E and E' formulated above we find

$$\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0) = -2\pi i\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle\,. \tag{3.74}$$

It yields

$$S^{(0)}_{\gamma_f,b;e_i,a} = -2\pi i\delta(E_b + k_f^0 - E_a - p_i^0)\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle \tag{3.75}$$

or according to the definition (3.2)

$$\tau^{(0)}_{\gamma_f,b;e_i,a} = -\langle b_2|e\alpha_\nu A^{\nu *}_f|p\rangle\,. \tag{3.76}$$

The corresponding cross section is

$$\frac{d\sigma^{(0)}}{d\Omega_f} = \frac{(2\pi)^4}{v_i}\,\mathbf{k}_f^2\,|\tau^{(0)}_{\gamma_f,b;e_i,a}|^2\,, \tag{3.77}$$

where v_i is the velocity of the incident electron in the nucleus frame.

2. Interelectronic-interaction corrections of first order in 1/Z

The interelectronic-interaction corrections of first order in $1/Z$ are defined by diagrams shown in Fig. 33. The formula (3.65) gives in the order under consideration

$$\begin{aligned} S^{(1)}_{\gamma_f,b;e_i,a} = \delta(E_b + k_f^0 - E_a - p_i^0)\,\Big[\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(1)}_{\gamma_f,b;e_i,a}(E',E,p_i^0) \\ -\frac{1}{2}\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\,\frac{1}{2\pi i}\oint_{\Gamma_b} dE\, g^{(1)}_{bb}(E)\Big]\,, \end{aligned} \tag{3.78}$$

where $g^{(1)}_{bb}(E)$ is defined by the first-order interelectronic-interaction diagram (see Fig. 20). According to the definition (3.66) and the Feynman rules we have

$$\begin{aligned} &g^{(1)}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\delta(E'+k^0-E-p_i^0) \\ &= \Big(\frac{i}{2\pi}\Big)^2 \sum_P (-1)^P \int_{-\infty}^{\infty} dp_1'^0 dp_2'^0 \delta(E'-p_1'^0-p_2'^0) \\ &\times \frac{1}{p_1'^0-\varepsilon_{Pb_1}+i0}\,\frac{1}{p_2'^0-\varepsilon_{Pb_2}+i0}\,\frac{1}{E-\varepsilon_a+i0}\int_{-\infty}^{\infty} dq^0 d\omega \\ &\times \sum_n \Big[\langle Pb_1Pb_2|I(\omega)|an\rangle\delta(p_2'^0+\omega-q^0)\delta(p_1'^0-\omega-E) \\ &\times \frac{1}{q^0-\varepsilon_n(1-i0)}\langle n|e\alpha_\nu A^{\nu *}_f|p\rangle\delta(q^0+k^0-p_i^0) \\ &+\langle Pb_1Pb_2|I(\omega)|np\rangle\delta(p_2'^0+\omega-p_i^0)\delta(p_1'^0-\omega-q^0) \\ &\times \frac{1}{q^0-\varepsilon_n(1-i0)}\langle n|e\alpha_\nu A^{\nu *}_f|a\rangle\delta(q^0+k^0-E) \\ &+\langle Pb_2|e\alpha_\nu A^{\nu *}_f|n\rangle\frac{1}{q^0-\varepsilon_n(1-i0)}\delta(p_2'^0+k^0-q^0) \\ &\times\langle Pb_1n|I(\omega)|ap\rangle\delta(q^0+\omega-p_i^0)\delta(p_1'^0-\omega-E) \\ &+\langle Pb_1|e\alpha_\nu A^{\nu *}_f|n\rangle\frac{1}{q^0-\varepsilon_n(1-i0)}\delta(p_1'^0+k^0-q^0) \\ &\times\langle nPb_2|I(\omega)|ap\rangle\delta(p_2'^0+\omega-p_i^0)\delta(q^0-\omega-E)\Big]\,. \end{aligned} \tag{3.79}$$

It yields

$$\begin{aligned} g^{(1)}_{\gamma_f,b;e_i,a}(E',E,p_i^0) = \Big(\frac{i}{2\pi}\Big)^2 \frac{1}{E'-E_b^{(0)}}\,\frac{1}{E-\varepsilon_a}\sum_P (-1)^P \sum_n \int_{-\infty}^{\infty} dp_1'^0 \\ \times\Big(\frac{1}{p_1'^0-\varepsilon_{Pb_1}+i0}+\frac{1}{E'-p_1'^0-\varepsilon_{Pb_2}+i0}\Big) \\ \times\Big[\langle Pb_1Pb_2|I(p_1'^0-E)|an\rangle\frac{1}{E'-E-\varepsilon_n(1-i0)}\langle n|e\alpha_\nu A^{\nu *}_f|p\rangle \\ +\langle Pb_2|e\alpha_\nu A^{\nu *}_f|n\rangle\frac{1}{E+p_i^0-p_1'^0-\varepsilon_n(1-i0)} \end{aligned}$$

$$
\begin{aligned}
&\times\langle Pb_1 n|I(p_1'^0-E)|ap\rangle\Big]\\
&+\Big(\frac{i}{2\pi}\Big)^2\frac{1}{E'-E_b^{(0)}}\frac{1}{E-\varepsilon_a}\sum_P(-1)^P\sum_n\int_{-\infty}^{\infty}dp_2'^0\\
&\times\Big(\frac{1}{p_2'^0-\varepsilon_{Pb_2}+i0}+\frac{1}{E'-p_2'^0-\varepsilon_{Pb_1}+i0}\Big)\\
&\times\Big[\langle Pb_1Pb_2|I(p_i^0-p_2'^0)|np\rangle\frac{1}{E'-p_i^0-\varepsilon_n(1-i0)}\langle n|e\alpha_\nu A_f^{\nu*}|a\rangle\\
&+\langle Pb_1|e\alpha_\nu A_f^{\nu*}|n\rangle\frac{1}{E+p_i^0-p_2'^0-\varepsilon_n(1-i0)}\\
&\times\langle nPb_2|I(p_i^0-p_2'^0)|ap\rangle\Big]\,. \qquad (3.80)
\end{aligned}
$$

The first term in equation (3.80) is conveniently devided into irreducible ($\varepsilon_n\neq E_b^{(0)}-\varepsilon_a=\varepsilon_{b_2}$) and reducible ($\varepsilon_n=\varepsilon_{b_2}$) parts. Since we consider the case of a single final state described by the one-determinant wave function (3.70) with $|b_1\rangle=|a\rangle$, the condition $\varepsilon_n=\varepsilon_{b_2}$ means $|n\rangle=|b_2\rangle$ (otherwise $\langle Pb_1Pb_2|I(\omega)|an\rangle=0$). Substituting (3.80) into (3.78), integrating over E and E' according to the rule formulated above and using the identity (2.127), one finds for the irreducible contribution

$$
\begin{aligned}
S^{(1,\mathrm{irred})}_{\gamma_f,b;e_i,a}&=\delta(E_b+k_f^0-E_a-p_i^0)\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\,g^{(1,\mathrm{irred})}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\\
&=-2\pi i\delta(E_b+k_f^0-E_a-p_i^0)\sum_P(-1)^P\\
&\quad\times\Big[\sum_n^{n\neq b_2}\langle Pb_1Pb_2|I(\varepsilon_{Pb_1}-\varepsilon_a)|an\rangle\frac{1}{\varepsilon_{b_2}-\varepsilon_n}\langle n|e\alpha_\nu A_f^{\nu*}|p\rangle\\
&\quad+\sum_n\langle Pb_2|e\alpha_\nu A_f^{\nu*}|n\rangle\frac{1}{\varepsilon_a+p_i^0-\varepsilon_{Pb_1}-\varepsilon_n}\langle Pb_1n|I(\varepsilon_{Pb_1}-\varepsilon_a)|ap\rangle\\
&\quad+\sum_n\langle Pb_1Pb_2|I(p_i^0-\varepsilon_{Pb_2})|np\rangle\frac{1}{E_b^{(0)}-p_i^0-\varepsilon_n}\langle n|e\alpha_\nu A_f^{\nu*}|a\rangle\\
&\quad+\sum_n\langle Pb_1|e\alpha_\nu A_f^{\nu*}|n\rangle\frac{1}{\varepsilon_a+p_i^0-\varepsilon_{Pb_2}-\varepsilon_n}\langle nPb_2|I(p_i^0-\varepsilon_{Pb_2})|ap\rangle\Big]\,. \qquad (3.81)
\end{aligned}
$$

For the reducible part we have

$$
\begin{aligned}
&\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\,g^{(1,\mathrm{red})}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\\
&=2\pi i\Big(\frac{i}{2\pi}\Big)^2\oint_{\Gamma_b}dE'\sum_P(-1)^P\frac{1}{(E'-E_b^{(0)})^2}\int_{-\infty}^{\infty}dp_1'^0\Big(\frac{1}{p_1'^0-\varepsilon_{Pb_1}+i0}\\
&+\frac{1}{E'-p_1'^0-\varepsilon_{Pb_2}+i0}\Big)\langle Pb_1Pb_2|I(p_1'^0-\varepsilon_a)|ab_2\rangle\langle b_2|e\alpha_\nu A_f^{\nu*}|p\rangle\\
&=-\sum_P(-1)^P\int_{-\infty}^{\infty}d\omega\frac{1}{(\omega-\varepsilon_{Pb_1}-i0)^2}\langle Pb_1Pb_2|I(\omega-\varepsilon_a)|b_1b_2\rangle\langle b_2|e\alpha_\nu A_f^{\nu*}|p\rangle\,. \qquad (3.82)
\end{aligned}
$$

The reducible contribution must be considered together with the second term in formula (3.78). Taking into account that

$$
\begin{aligned}
\frac{1}{2\pi i}\oint_{\Gamma_b}dEg_{bb}^{(1)}(E)=-\frac{i}{2\pi}\Big[&2\int_{-\infty}^{\infty}dp_1'^0\frac{1}{(p'^0-\varepsilon_{b_1}-i0)^2}\langle b_1b_2|I(p_1'^0-\varepsilon_{b_1})|b_1b_2\rangle\\
&-\int_{-\infty}^{\infty}dp_1'^0\frac{1}{(p_1'^0-\varepsilon_{b_2}-i0)^2}\langle b_2b_1|I(p_1'^0-\varepsilon_{b_1})|b_1b_2\rangle\\
&-\int_{-\infty}^{\infty}dp_1^0\frac{1}{(p_1^0-\varepsilon_{b_1}-i0)^2}\langle b_2b_1|I(p_1^0-\varepsilon_{b_2})|b_1b_2\rangle \qquad (3.83)
\end{aligned}
$$

one finds

$$
\begin{aligned}
&-\frac{1}{2}\oint_{\Gamma_b} dE' \oint_{\Gamma_a} dE\, g^{(0)}_{\gamma_f,b;e_i,a}(E',E,p_i^0)\frac{1}{2\pi i}\oint_{\Gamma_b} dE g^{(1)}_{bb}(E)\\
&=\frac{1}{2}\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle\Big[2\int_{-\infty}^{\infty} d\omega \frac{\langle b_1 b_2|I(\omega)|b_1 b_2\rangle}{(\omega-i0)^2}\\
&-\int_{-\infty}^{\infty} d\omega\langle b_2 b_1|I(\omega)|b_1 b_2\rangle\Big(\frac{1}{(\omega-\Delta_b-i0)^2}+\frac{1}{(\omega+\Delta_b-i0)^2}\Big)\Big]\,, \qquad (3.84)
\end{aligned}
$$

where $\Delta_b \equiv \varepsilon_{b_2}-\varepsilon_{b_1}$. Summing (3.82) and (3.84), we obtain for the total reducible contribution

$$
\begin{aligned}
S^{(1,\mathrm{red})}_{\gamma_f,b;e_i,a} &= -2\pi i\delta(E_b+k_f^0-E_a-p_i^0)\frac{1}{2}\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\langle b_2 b_1|I(\omega)|b_1 b_2\rangle\\
&\times\Big[\frac{1}{(\omega+\Delta_b+i0)^2}-\frac{1}{(\omega+\Delta_b-i0)^2}\Big]\,. \qquad (3.85)
\end{aligned}
$$

Using the identity

$$
\frac{1}{(\omega+i0)^2}-\frac{1}{(\omega-i0)^2}=-\frac{2\pi}{i}\frac{d}{d\omega}\delta(\omega) \qquad (3.86)
$$

and integrating by parts we find

$$
S^{(1,\mathrm{red})}_{\gamma_f,b;e_i,a} = 2\pi i\delta(E_b+k_f^0-E_a-p_i^0)\frac{1}{2}\langle b_2|e\alpha_\nu A_f^{\nu *}|p\rangle\langle b_2 b_1|I'(\Delta_b)|b_1 b_2\rangle\,. \qquad (3.87)
$$

In addition to the interelectronic-interaction correction derived in this subsection, we must take into account the contribution originating from changing the photon energy in the zeroth-order cross section (3.77) due to the interelectronic-interaction correction to the energy of the bound state b. It follows that the total interelectronic-interaction correction of first order in $1/Z$ to the cross section is given by

$$
\frac{d\sigma^{(1)}}{d\Omega_f}=\frac{(2\pi)^4}{v_i}\mathbf{k}_f^2\,2\mathrm{Re}\Big\{\tau^{(0)*}_{\gamma_f,b;e_i,a}\tau^{(1)}_{\gamma_f,b;e_i,a}\Big\}+\Big[\frac{d\sigma^{(0)}}{d\Omega_f}\Big|_{k_f^0=p_i^0+\varepsilon_a-E_b}-\frac{d\sigma^{(0)}}{d\Omega_f}\Big|_{k_f^0=p_i^0+\varepsilon_a-E_b^{(0)}}\Big]\,. \qquad (3.88)
$$

Here $\tau^{(1)}_{\gamma_f,b;e_i,a}=\tau^{(1,\mathrm{irred})}_{\gamma_f,b;e_i,a}+\tau^{(1,\mathrm{red})}_{\gamma_f,b;e_i,a}$ is the interelectronic-interaction correction given by equations (3.81) and (3.87) in accordance with the definition (3.2). E_b and $E_b^{(0)}$ are the energies of the bound state b with and without the interelectronic-interaction correction, respectively.

E. Photon scattering on an atom

Let us consider the scattering of a photon with momentum $\mathbf{k}_i$ and polarization $\epsilon_i=(0,\boldsymbol{\epsilon}_i)$ on an atom being initially in a state a. As a result of the scattering, a photon with momentum $\mathbf{k}_f$ and polarization $\epsilon_f=(0,\boldsymbol{\epsilon}_f)$ arises and the atom comes to a state b. In this section we consider the non-resonance photon scattering. This means that the total initial energy of the system $(E_a+k_i^0)$ is not close to any excited state energy of the atom. The resonance photon scattering will be considered in detail in the next section.

According to the standard reduction technique (see, e.g., [24]), the amplitude of the process is

$$
\begin{aligned}
S_{\gamma_f,b;\gamma_i,a} &= \langle b|a_{\mathrm{out}}(k_f,\epsilon_f)a^\dagger_{\mathrm{in}}(k_i,\epsilon_i)|a\rangle\\
&=\mathrm{Disconnected\ \ term}-Z_3^{-1}\int d^4y d^4z\frac{\epsilon_f^\nu\exp\left(ik_f\cdot y\right)}{\sqrt{2k_f^0(2\pi)^3}}\\
&\times\langle b|Tj_\nu(y)j_\rho(z)|a\rangle\frac{\epsilon_i^\rho\exp\left(-ik_i\cdot z\right)}{\sqrt{2k_i^0(2\pi)^3}}\,, \qquad (3.89)
\end{aligned}
$$

where $|a\rangle$ and $|b\rangle$ are the vectors of the initial and final states in the Heisenberg representation; $k_f=(k_f^0,\mathbf{k}_f)$ and $k_i=(k_i^0,\mathbf{k}_i)$. The first term in the right-hand side of equation (3.89) corresponds to a non-scattering process (the

photon does not interact with the atom). We are interested in the second term which describes the photon scattering on the atom. Let us designate this term by $S^{\rm scat}_{\gamma_f,b;\gamma_i,a}$.

To derive the calculation formula for $S^{\rm scat}_{\gamma_f,b;\gamma_i,a}$ we isolate in the scattering amplitude a term which describes the scattering of the photon by the Coulomb potential $V_{\rm C}$. With this in mind, we write

$$\langle b|Tj(y)j(z)|a\rangle = \langle b|[Tj(y)j(z) - \langle 0|Tj(y)j(z)|0\rangle]|a\rangle + \delta_{ab}\langle 0|Tj(y)j(z)|0\rangle\,. \tag{3.90}$$

The second term in the right-hand side of this equation corresponds to the photon scattering by the Coulomb field and the first term describes the photon scattering by the atomic electrons. Since only diagrams in which the incident photon is connected at least with one external electron line contribute to the first term, we denote this term by $S^{\rm con}_{\gamma_f,b;\gamma_i,a}$. We have

$$\begin{aligned}
S^{\rm con}_{\gamma_f,b;\gamma_i,a} &= -Z_3^{-1}\int d^4y d^4z \frac{\epsilon_f^\nu \exp(ik_f\cdot y)}{\sqrt{2k_f^0(2\pi)^3}}\langle b|[Tj_\nu(y)j_\rho(z)\\
&\quad -\langle 0|Tj_\nu(y)j_\rho(z)|0\rangle]|a\rangle\frac{\epsilon_i^\rho \exp(-ik_i\cdot z)}{\sqrt{2k_i^0(2\pi)^3}}\\
&= -Z_3^{-1}2\pi\delta(E_b+k_f^0-E_a-k_i^0)\int_{-\infty}^{\infty}dt\exp(ik_f^0t)\int d\mathbf{y}d\mathbf{z}A_f^{\nu *}(\mathbf{y})\\
&\quad\times\langle b|[Tj_\nu(t,\mathbf{y})j_\rho(0,\mathbf{z}) - \langle 0|Tj_\nu(t,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]|a\rangle A_i^\rho(\mathbf{z})\,.
\end{aligned} \tag{3.91}$$

Here the second term is zero if $a\neq b$.

To construct the perturbation theory for the amplitude of the process we introduce the Fourier transform of the corresponding two-time Green function

$$\begin{aligned}
&\mathcal{G}^{\rm con}_{\gamma_f;\gamma_i}(E',E,k'^0;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_N)\delta(E'+k'^0-E-k^0)\\
&=\Big(\frac{i}{2\pi}\Big)^2\frac{1}{N!}\int_{-\infty}^{\infty}dx^0dx'^0\int d^4yd^4z\ \exp(iE'x'^0+ik'^0y^0-iEx^0-ik^0z^0)\\
&\quad\times A_f^{\nu *}(\mathbf{y})A_i^\rho(\mathbf{z})\langle 0|T\psi(x'^0,\mathbf{x}'_1)\cdots\psi(x'^0,\mathbf{x}'_N)[j_\nu(y)j_\rho(z)\\
&\quad-\langle 0|Tj_\nu(y)j_\rho(z)|0\rangle]\overline{\psi}(x^0,\mathbf{x}_N)\cdots\overline{\psi}(x^0,\mathbf{x}_1)|0\rangle\,.
\end{aligned} \tag{3.92}$$

Introducing $t'=x'^0-z^0,\ t=x^0-z^0$, and $\tau=y^0-z^0$ and integrating over z^0 we obtain

$$\begin{aligned}
&\mathcal{G}^{\rm con}_{\gamma_f;\gamma_i}(E',E,k'^0;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_N)\delta(E'+k'^0-E-k^0)\\
&=-\delta(E'+k'^0-E-k^0)\frac{1}{2\pi}\frac{1}{N!}\int_{-\infty}^{\infty}dtdt'd\tau\exp(iE't'+ik'^0\tau-iE\tau)\\
&\quad\times\int d\mathbf{y}d\mathbf{z}A_f^{\nu *}(\mathbf{y})A_i^\rho(\mathbf{z})\langle 0|T\psi(t',\mathbf{x}'_1)\cdots\psi(t',\mathbf{x}'_N)[j_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})\\
&\quad-\langle 0|Tj_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]\overline{\psi}(t,\mathbf{x}_N)\cdots\overline{\psi}(t,\mathbf{x}_1)|0\rangle\,.
\end{aligned} \tag{3.93}$$

Integrating over t and t' we find

$$\begin{aligned}
&\mathcal{G}^{\rm con}_{\gamma_f;\gamma_i}(E',E,k'^0;\mathbf{x}'_1,...\mathbf{x}'_N;\mathbf{x}_1,...\mathbf{x}_N)\\
&=-\frac{1}{2\pi}\frac{1}{N!}\sum_{n,m}\frac{i}{E'-E_n+i0}\frac{i}{E-E_m+i0}\int_{-\infty}^{\infty}d\tau\exp(ik'^0\tau)\\
&\quad\times\int d\mathbf{y}d\mathbf{z}A_f^{\nu *}(\mathbf{y})A_i^\rho(\mathbf{z})\{\theta(\tau)\exp[i\tau(E'-E_n)]\langle 0|T\psi(0,\mathbf{x}'_1)\cdots\psi(0,\mathbf{x}'_N)|n\rangle\\
&\quad\times\langle n|[j_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})-\langle 0|Tj_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]|m\rangle\\
&\quad\times\langle m|\overline{\psi}(0,\mathbf{x}_N)\cdots\overline{\psi}(0,\mathbf{x}_1)|0\rangle+\theta(-\tau)\exp[i\tau(E_m-E)]\\
&\quad\times\langle 0|T\psi(0,\mathbf{x}'_1)\cdots\psi(0,\mathbf{x}'_N)|n\rangle\langle n|[j_\rho(0,\mathbf{z})j_\nu(\tau,\mathbf{y})\\
&\quad-\langle 0|Tj_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]|m\rangle\langle m|\overline{\psi}(0,\mathbf{x}_N)\cdots\overline{\psi}(0,\mathbf{x}_1)|0\rangle+\cdots\}\,.
\end{aligned} \tag{3.94}$$

It can be shown that the terms which are omitted in equation (3.94) are regular functions of E' or E when $E'\approx E_b$ and $E\approx E_a$. As in the previous sections of this paper, we assume that in the zeroth approximation the initial and

final states of the atom are degenerate in energy with some other states and use the same notations for these states as above. As usual, we also assume that a non-zero photon mass μ is introduced. We define the Green function $g^{\rm con}_{\gamma_f,b;\gamma_i,a}(E',E,k'^0)$ by

$$g_{\gamma_f,b;\gamma_i,a}(E',E,k'^0)=P_b^{(0)}\mathcal{G}^{\rm con}_{\gamma_f;\gamma_i}(E',E,k'^0)\gamma_1^0\cdots\gamma_N^0P_a^{(0)}\,. \tag{3.95}$$

From equation (3.94) we have

$$\begin{aligned}g^{\rm con}_{\gamma_f,b;\gamma_i,a}(E',E,k'^0)=&\frac{1}{2\pi}\sum_{n_a,n_b}\frac{\varphi_{n_b}}{E'-E_{n_b}}\int d\mathbf{y}d\mathbf{z}A_f^{\nu*}(\mathbf{y})A_i^{\rho}(\mathbf{z})\int_{-\infty}^{\infty}d\tau\exp\left(ik'^0\tau\right)\\
&\times\{\theta(\tau)\exp\left[i\tau(E'-E_{n_b})\right]\langle n_b|[j_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})\\
&-\langle0|Tj_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]|n_a\rangle+\theta(-\tau)\exp\left[i\tau(E_{n_a}-E)\right]\\
&\times\langle n_b|[j_\rho(0,\mathbf{z})j_\nu(\tau,\mathbf{y})-\langle0|Tj_\nu(\tau,\mathbf{y})j_\rho(0,\mathbf{z})|0\rangle]|n_a\rangle\}\frac{\varphi^\dagger_{n_a}}{E-E_{n_a}}\\
&+\text{ terms that are regular functions of }E'\text{ or }E\text{ when }E'\approx E_b^{(0)}\\
&\quad\text{and }E\approx E_a^{(0)}\,.\end{aligned} \tag{3.96}$$

Taking into account the biorthogonality condition (2.71) and comparing (3.91) with (3.96) we get the desirable formula [26]

$$S^{\rm con}_{\gamma_f,b;\gamma_i,a}=Z_3^{-1}\delta(E_b+k_f^0-E_a-k_i^0)\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dE\;v_b^\dagger g^{\rm con}_{\gamma_f,b;\gamma_i,a}(E',E,k_f^0)v_a\,, \tag{3.97}$$

where we imply by a one of the initial states and by b one of the final states under consideration. In the case of a single initial state (a) and a single final state (b) it yields

$$\begin{aligned}S^{\rm con}_{\gamma_f,b;\gamma_i,a}=&Z_3^{-1}\delta(E_b+k_f^0-E_a-k_i^0)\oint_{\Gamma_b}dE'\oint_{\Gamma_a}dEg^{\rm con}_{\gamma_f,b;\gamma_i,a}(E',E,k_f^0)\\
&\times\Big[\frac{1}{2\pi i}\oint_{\Gamma_b}dEg_{bb}(E)\Big]^{-1/2}\Big[\frac{1}{2\pi i}\oint_{\Gamma_a}dEg_{aa}(E)\Big]^{-1/2}.\end{aligned} \tag{3.98}$$

The disconnected term describing the scattering of the photon by the Coulomb field is calculated by the formula

$$S^{\rm discon}_{\gamma_f,b;\gamma_i,a}=-Z_3^{-1}\delta_{ab}\int d^4yd^4z\frac{\epsilon_f^\nu\exp\left(ik_f\cdot y\right)}{\sqrt{2k_f^0(2\pi)^3}}\langle0|Tj_\nu(y)j_\rho(z)|0\rangle\frac{\epsilon_i^\rho\exp\left(-ik_i\cdot z\right)}{\sqrt{2k_i^0(2\pi)^3}}\,. \tag{3.99}$$

For practical calculations by perturbation theory it is convenient to express the Green function $g^{\rm con}_{\gamma_f,b;\gamma_i,a}$ in terms of the Fourier transform of the $2N$-time Green function

$$\begin{aligned}&g^{\rm con}_{\gamma_f,b;\gamma_i,a}(E',E,k'^0)\delta(E'+k'^0-E-k^0)\\
&=\frac{1}{N!}\int_{-\infty}^{\infty}dp_1^0\cdots dp_N^0dp_1'^0\cdots dp_N'^0\;\delta(E-p_1^0\cdots-p_N^0)\delta(E'-p_1'^0\cdots-p_N'^0)\\
&\times P_b^{(0)}G^{\rm con}_{\gamma_f;\gamma_i}(p_1'^0,...,p_N'^0;k'^0,k^0;p_1^0,...,p_N^0)\gamma_1^0\cdots\gamma_N^0P_a^{(0)}\,,\end{aligned} \tag{3.100}$$

where

$$\begin{aligned}&G^{\rm con}_{\gamma_f;\gamma_i}((p_1'^0,\mathbf{x}_1'),...,(p_N'^0,\mathbf{x}_N');k'^0,k^0;(p_1^0,\mathbf{x}_1),...,(p_N^0,\mathbf{x}_N))\\
&=-\frac{1}{(2\pi)^{2N}}\int_{-\infty}^{\infty}dx_1^0\cdots dx_N^0dx_1'^0\cdots dx_N'^0\\
&\times\exp\left(ip_1'^0x_1'^0+\cdots+ip_N'^0x_N'^0-ip_1^0x_1^0-\cdots-ip_N^0x_N^0\right)\\
&\times\int d^4yd^4z\exp\left(ik'^0y^0-ik^0z^0\right)A_f^{\nu*}(\mathbf{y})\\
&\times\langle0|T\psi(x_1')\cdots\psi(x_N')[j_\nu(y)j_\rho(z)-\langle0|Tj_\nu(y)j_\rho(z)|0\rangle]\\
&\times\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle A_i^\rho(\mathbf{z})\,.\end{aligned} \tag{3.101}$$

The Green function $G^{\rm con}_{\gamma_f,\gamma_i}$ is constructed using Wick's theorem after the transition in (3.101) to the interaction representation. The Feynman rules for $G^{\rm con}_{\gamma_f,\gamma_i}$ differ from those for G_{γ_f} only by presence of the incoming photon line which corresponds to the incident photon wave function $A_i^\rho(\mathbf{x})$.

F. Resonance scattering: Spectral line shape

The formulas for the scattering amplitudes derived above allow one to perform calculations by perturbation theory in the case when the total initial energy of the system is not close to the energy of an intermediate quasistationary state. This is so-called non-resonance scattering. In the case of the resonance scattering, when the initial energy of the system is close to an intermediate state energy, the direct calculation by perturbation theory according to the formulas derived above leads to some singularities in the scattering amplitude. It means that these formulas can not be directly applied to the resonance processes. In this section we formulate a method which allows one to calculate the resonance scattering amplitudes. This method was worked out in Ref. [29]. Another approach, which is limited to the one-electron atom case, was previously developed in Ref. [75]. An attempt to describe a decay process within QED was undertaken in Ref. [76].

Let us consider the photon scattering on an atom being initially in its ground state "a" in the case of resonance $E_a + k_i^0 \sim E_d (d = 1, ..., s)$, where E_a is the ground state energy of the atom, k_i^0 is the incident photon energy, and $E_d (d = 1, ..., s)$ are the energies of intermediate atomic states which in zeroth order approximation are equal to the unperturbed energy $E_d^{(0)}$ of a degenerate level. We consider that, as a result of the scattering, a photon of energy $k_f^0 = k_i^0$ is emitted and the atom comes again to its ground state a. The calculation of the photon scattering amplitude by the formula derived above leads to a singularity which is caused by the fact that in a finite order of the perturbation theory one of the energy denominators of an intermediate Green function is close to zero. It means that in the calculation of the Green function $g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0)$ we have to go beyond the finite order approximation. With this in mind, let us represent $g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0)$ as

$$g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0) = \frac{i}{2\pi} g_a(E') R^{(-)}_{\gamma_f}(E', k'^0, E + k^0) \frac{i}{2\pi} g_d(E + k^0) R^{(+)}_{\gamma_i}(E + k^0, k^0, E) \frac{i}{2\pi} g_a(E) + \Delta g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0)\,, \tag{3.102}$$

where g_a are g_d are the Green function defined by equation (2.63) with the projectors $P_a^{(0)}$ and $P_d^{(0)}$, respectively, $k^0 = k'^0 + E' - E$, and $\Delta g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0)$ is a part of the Green function $g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k'^0)$ which is regular at $E + k^0 \sim E_d (d = 1, ..., s)$. The operators $R^{(-)}_{\gamma_f}$ and $R^{(+)}_{\gamma_i}$ are constructed by perturbation theory from equation (3.102) which must be considered as their definition. Taking into account equation (2.64) und using the formula (3.97) we obtain

$$S^{\rm con}_{\gamma_f,a;\gamma_i,a} = Z_3^{-1} \delta(k_f^0 - k_i^0) \varphi_a^\dagger R^{(-)}_{\gamma_f}(E_a, k_f^0, E_a + k_i^0) \frac{i}{2\pi} g_d(E_a + k_i^0) R^{(+)}_{\gamma_i}(E_a + k_i^0, k_i^0, E_a) \varphi_a + Z_3^{-1} \delta(k_f^0 - k_i^0) \oint_{\Gamma_a} dE' \oint_{\Gamma_a} dE v_a^\dagger \Delta g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E', E, k_f^0) v_a\,. \tag{3.103}$$

Consider now how the intermediate Green function $g_d(E_a + k_i^0)$ can be calculated. Let us introduce a quasipotential $V_d(E)$ by

$$g_d(E) = g_d^{(0)}(E) + g_d^{(0)}(E) V_d(E) g_d(E)\,, \tag{3.104}$$

where $g_d^{(0)} = P_d^{(0)}/(E - E_d^{(0)})$. The quasipotential $V_d(E)$ is constructed by perturbation theory according to equation (3.104) which must be considered as its definition. This equation yields

$$V_d(E) = [g_d^{(0)}(E)]^{-1} - [g_d(E)]^{-1} = [g_d^{(0)}(E)]^{-1} - [g_d^{(0)}(E) + g_d^{(1)}(E) + \cdots]^{-1} = [g_d^{(0)}(E)]^{-1} g_d^{(1)}(E) [g_d^{(0)}(E)]^{-1} + \cdots\,. \tag{3.105}$$

When the quasipotential $V_d(E)$ is constructed from equation (3.105) to a finite order of the perturbation theory, the Green function g_d is determined by

$$g_d(E) = [E - E_d^{(0)} - V_d(E)]^{-1}\,. \tag{3.106}$$

The Green function $g_d(E)$ has poles on the second sheet of the Riemann surface, slightly below the right-hand real semiaxis (see Fig. 5), and has no singularities for real E when $E \sim E_d^{(0)}$. It means, in particular, that if we take the quasipotential at least to the lowest order approximation ($V(E) \approx V(E_d^{(0)})$), the Green function $g_d(E)$ calculated by equation (3.106) has no singularities at $E \sim E_d (d = 1, ..., s)$, and, therefore, the calculation of the resonance scattering

amplitude by equation (3.103) will be correct. The calculation of $g_d(E)$ by equation (3.106) corresponds effectively to summing an infinite subsequence of Feynman diagrams.

For calculation of $g_d(E)$ to the lowest order approximation it is convenient to introduce an operator $\mathcal{H}$ by

$$\mathcal{H} \equiv E_d^{(0)} + V_d(E_d^{(0)})\,. \tag{3.107}$$

The operator $\mathcal{H}$ is not Hermitian and has complex eigenvalues. We assume that $\mathcal{H}$ is a simple matrix, i.e. its eigenvectors form a full basis in the space of the unperturbed d-states. We denote its eigenvalues by $\mathcal{E}_d = E_d - i\Gamma_d/2$, the right eigenvectors by $|d_R\rangle$, and the left eigenvectors by $|d_L\rangle$. It means

$$\mathcal{H}|d_R\rangle = \mathcal{E}_d|d_R\rangle\,, \qquad \langle d_L|\mathcal{H} = \langle d_L|\mathcal{E}_d\,. \tag{3.108}$$

It is convenient to normalize the vectors $|d_R\rangle$, $|d_L\rangle$ by the condition

$$\langle d_L|d'_R\rangle = \delta_{dd'}\,. \tag{3.109}$$

They satisfy the completeness condition

$$\sum_{d=1}^{s} |d_R\rangle\langle d_L| = I\,. \tag{3.110}$$

For $g_d(E)$ we obtain

$$g_d(E) \approx (E-\mathcal{H})^{-1} = \sum_{d=1}^{s} \frac{|d_R\rangle\langle d_L|}{E-\mathcal{E}_d}\,. \tag{3.111}$$

In fact, due to T-invariance $\mathcal{H}_{ik} = \mathcal{H}_{ki}$. For this reason the components of the vector $\langle d_L|$ can be chosen to be equal to the corresponding components of the vector $|d_R\rangle$. In other words, the components of the vector $|d_R\rangle$ are equal to the complex conjugated components of the vector $|d_L\rangle$. If among the d states there are ones with different quantum numbers, such as the total angular momentum or the parity, for them we have $|d_R\rangle = |d_L\rangle \equiv |d\rangle$.

Substituting the lowest order approximation for $g_d(E)$ given by equation (3.111) into (3.103) we obtain in the resonance approximation

$$S^{\rm con}_{\gamma_f,a;\gamma_i,a} \approx \frac{i}{2\pi}\delta(k_f^0-k_i^0)\sum_{d=1}^{s}\frac{\langle a|R^{(-)}_{\gamma_f}|d_R\rangle\langle d_L|R^{(+)}_{\gamma_i}|a\rangle}{E_a+k_i^0-E_d+i\Gamma_d/2}\,. \tag{3.112}$$

In the resonance approximation, it is sufficient to evaluate the operators $R^{(-)}_{\gamma_f}$, $R^{(+)}_{\gamma_i}$ to the lowest order of the perturbation theory. They are determined directly from equation (3.102).

To demonstrate how the method works we consider below the resonance photon scattering on a one-electron atom. A more general case of a few-electron atom is considered in [29].

G. Resonance photon scattering on a one-electron atom

In the lowest order the photon scattering on a one-electron atom is described by the diagram shown in Fig. 34. The contribution of this diagram to the Green function G_{γ_f,γ_i} is

$$\begin{aligned} G^{\rm con}_{\gamma_f,\gamma_i}((E',\mathbf{x}');k'^0,k^0;(E,\mathbf{x})) = \int d\mathbf{y}d\mathbf{z}\int_{-\infty}^{\infty} dp^0 \frac{i}{2\pi}S(E',\mathbf{x}',\mathbf{y})\frac{2\pi}{i}e\gamma_\nu\delta(E'+k'^0-p^0) \\ \times A_f^{\nu *}(\mathbf{y})\frac{i}{2\pi}S(p^0,\mathbf{y},\mathbf{z})\frac{2\pi}{i}e\gamma_\rho\delta(p^0-k^0-E) \\ \times A_i^{\rho}(\mathbf{z})\frac{i}{2\pi}S(E,\mathbf{z},\mathbf{x})\,. \end{aligned} \tag{3.113}$$

For $g^{\rm con}_{\gamma_f,a;\gamma_i,a}$ one finds

$$g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E',E,k'^0) = \frac{i}{2\pi}\frac{|a\rangle\langle a|}{E'-\varepsilon_a}\frac{2\pi}{i}e\alpha_\nu A^{\nu*}_f \times\frac{i}{2\pi}\sum_n \frac{|n\rangle\langle n|}{E+k^0-\varepsilon_n(1-i0)}\frac{2\pi}{i}e\alpha_\rho A^\rho_i\frac{i}{2\pi}\frac{|a\rangle\langle a|}{E-\varepsilon_a}\,. \tag{3.114}$$

We consider that $E_a+k^0_i\sim E_d$ and, therefore, represent $g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E',E,k'^0)$ as the sum of two terms

$$\begin{aligned} g^{\rm con}_{\gamma_f,a;\gamma_i,a}(E',E,k'^0) &= \frac{i}{2\pi}g^{(0)}_a(E')\frac{2\pi}{i}e\alpha_\nu A^{\nu*}_f\frac{i}{2\pi}g^{(0)}_d(E+k^0) \\ &\times\frac{2\pi}{i}e\alpha_\rho A^\rho_i\frac{i}{2\pi}g^{(0)}_a(E)+\frac{i}{2\pi}g^{(0)}_a(E')\frac{2\pi}{i}e\alpha_\nu A^{\nu*}_f \\ &\times\sum_n^{\varepsilon_n\neq\varepsilon_d}\frac{|n\rangle\langle n|}{E+k^0-\varepsilon_n(1-i0)}e\alpha_\rho A^\rho_i g^{(0)}_a(E)\,. \end{aligned} \tag{3.115}$$

Comparing this equation with equation (3.102) we derive

$$R^{(-)}_{\gamma_f}(\mathbf{y}) = \frac{2\pi}{i}e\alpha_\nu A^{\nu*}_f(\mathbf{y})\,, \qquad R^{(+)}_{\gamma_i}(\mathbf{z}) = \frac{2\pi}{i}e\alpha_\rho A^\rho_i(\mathbf{z})\,. \tag{3.116}$$

Let us derive now the quasipotential $V_d(E)$. To the lowest order of the perturbation theory it is defined by the SE and VP diagrams (see Figs. 12,13). As was derived above (see section II), the contribution of these diagrams to $g_d(E)$ is

$$g^{(1)}_d(E) = g^{(0)}_d(\Sigma_{\rm SE}(E)+U_{\rm VP})g^{(0)}_d. \tag{3.117}$$

Therefore,

$$V^{(1)}_d(E) = [g^{(0)}_d(E)]^{-1}g^{(1)}_d(E)[g^{(0)}_d(E)]^{-1} = P^{(0)}_d(\Sigma_{\rm SE}(E)+U_{\rm VP})P^{(0)}_d\,. \tag{3.118}$$

The operator $P^{(0)}_d\Sigma_{\rm SE}(E)P^{(0)}_d$ contains a non-Hermitian part which is responsible for the imaginary part of the energy. The operator

$$\mathcal{H} = \varepsilon_d + V^{(1)}_d(\varepsilon_a+k^0_i) \tag{3.119}$$

acts in the s-dimensional space of the unperturbed states. In reality, due to the fact that the operators $\Sigma_{\rm SE}$ and $U_{\rm VP}$ do not mix states with different quantum numbers and among the degenerate one-electron states there are no states with the same quantum numbers, in the case under consideration the right eigenvectors of $\mathcal{H}$ coincide with the left eigenvectors, $|d_R\rangle = |d_L\rangle \equiv |d\rangle$. However, to keep a general form of the equations we will use below the right and left eigenvectors. In the resonance approximation, the amplitude of the process is defined by equation (3.112), where the operators $R^{(-)}_{\gamma_f}$ and $R^{(+)}_{\gamma_i}$ are given by equations (3.116), $E_a=\varepsilon_a+\langle a|\Sigma_{\rm SE}(\varepsilon_a)+U_{\rm VP}|a\rangle$ is the ground state energy including the QED corrections of first order in α, E_d and $-\Gamma_d/2$ are the real and imaginary parts of an eigenvalue of $\mathcal{H}$.

For the differential cross section in the resonance approximation we obtain

$$\begin{aligned} d\sigma = (2\pi)^4\delta(k^0_f-k^0_i)\Big[&\sum_{d=1}^s\frac{|\langle a|e\alpha_\nu A^{\nu*}_f|d_R\rangle\langle d_L|e\alpha_\rho A^\rho_i|a\rangle|^2}{(E_a+k^0_i-E_d)^2+\Gamma^2_d/4} \\ &+2{\rm Re}\sum_{d<d'}\frac{\langle a|e\alpha_\nu A^{\nu*}_f|d_R\rangle\langle d_L|e\alpha_\rho A^\rho_i|a\rangle|^2}{E_a+k^0_i-E_d+i\Gamma_d/2} \\ &\times\frac{\langle a|e\alpha_\nu A^{\nu*}_f|d'_R\rangle^*\langle d'_L|e\alpha_\rho A^\rho_i|a\rangle^*}{E_a+k^0_i-E_{d'}-i\Gamma_{d'}/2}\Big]d\mathbf{k}_f\,. \end{aligned} \tag{3.120}$$

For the total cross section, using the optical theorem, we find

$$\begin{aligned} \sigma_{\rm tot} = 2(2\pi)^3\sum_{d=1}^s\Big[&\frac{{\rm Re}(\langle a|e\alpha_\nu A^{\nu*}_i|d_R\rangle\langle d_L|e\alpha_\rho A^\rho_i|a\rangle)(\Gamma_d/2)}{(E_a+k^0_i-E_d)^2+\Gamma^2_d/4} \\ &+\frac{{\rm Im}(\langle a|e\alpha_\nu A^{\nu*}_i|d_R\rangle\langle d_L|e\alpha_\rho A^\rho_i|a\rangle)(E_d-E_a-k^0_i)}{(E_a+k^0_i-E_d)^2+\Gamma^2_d/4}\Big]\,. \end{aligned} \tag{3.121}$$

Let us discuss, for simplicity, the case $s = 2$. The second term in the right-hand side of equation (3.121) is not equal to zero only if the levels ($d = 1, 2$) have the same quantum numbers. In the opposite case, which has place in the process under consideration, $|d_R\rangle = |d_L\rangle$ and, therefore,

$$\mathrm{Im}(\langle a|e\alpha_\nu A_i^{\nu *}|d\rangle\langle d|e\alpha_\rho A_i^\rho|a\rangle) = 0\,. \tag{3.122}$$

It follows that the the total cross section given by equation (3.121) is the sum of Lorentz-type terms. As to the differential cross section, the second term in equation (3.120) is non-zero even if the states $d = 1, 2$ have different quantum numbers.

Close levels with identical quantum numbers can appear among double excited states of high-Z few-electron atoms [77]. As those, we can consider the $(2s, 2s)_0$ and $(2p_{1/2}, 2p_{1/2})_0$ states of a He-like ion which can arise in the process of recombination of an electron with a H-like ion. A detailed theory of this process is given in Ref. [33]. The related calculations are presented in Refs. [30,78].

IV. CONCLUSION

In the present paper we considered in detail the two-time Green function method for high-Z few-electron systems. To demonstrate the efficiency of the method we derived formulas for some corrections to the energy levels, transition and scattering amplitudes in one-, two-, and three-electron atoms. Many other applications of the method can be found in Refs. [31–42,79]. In particular, in Refs. [38,39] the vacuum-polarization and self-energy screening corrections to the energies of lithiumlike ions are derived. The two-photon exchange diagrams for lithiumlike ions are evaluated in Ref. [79]. The second order two-electron diagrams for quasidegenerate states of heliumlike ions are studied in [40,68,80]. In Ref. [31], the TTGF method is employed to construct an effective energy operator for a high-Z few-electron atom. In Ref. [41], this method is used to derive the QED corrections to the radiative recombination of an electron with a bare nucleus. The interelectronic-interaction corrections to the radiative electron capture of an electron with a heliumlike ion are considered in [42]. In Ref. [73], the interelectronic-interaction corrections to the transition probabilities in heliumlike ions are derived.

Concluding, the two-time Green function method provides a uniform and very efficient approach for deriving the QED corrections to energy levels, transition probabilities, and cross sections of scattering processes in high-Z few-electron atoms. Using an effective potential instead of the Coulomb potential of the nucleus allows one to extend this approach to many-electron atoms.

ACKNOWLEDGEMENTS

Many practical calculations by the TTGF method were carried out in collaboration with Anton Artemyev and Vladimir Yerokhin. Stimulating discussions with T. Beier, E.-O. Le Bigot, J. Eichler, P. Indelicato, U. Jentschura, S. Karshenboim, I. Lindgren, P. Mohr, G. Plunien, J. Sapirstein, G. Soff, and S. Zschocke are gratefully acknoweldeged. This work was supported in part by RFBR (Grant No. 98-02-18350 and Grant No. 98-02-0411) and by the program "Russian Universities - Basic Research" (project No. 3930).

APPENDIX A

In the Heisenberg representation the basic equations of the quantum electrodynamics in presence of a classical time-independent field $A^{\nu}_{\rm cl}(\mathbf{x})$ are

$$(i\,\partial\!\!\!/ - m - e\,A\!\!\!/_{\rm cl}\,(\mathbf{x}))\psi(x) = e\,A\!\!\!/\,(x)\psi(x) - \delta m\psi(x)\,,$$
$$\Box A_{\nu}(x) = j_{\nu}(x)\,, \tag{A1}$$

where $j_{\nu}(x) = (e/2)[\overline{\psi}(x)\gamma_{\nu},\psi(x)]$ is the electron-positron current operator. The state vectors in the Heisenberg representation are time-independent

$$\partial_t|\Phi\rangle = 0\,. \tag{A2}$$

The physical state vectors have to obey a subsidiary condition

$$(\partial_{\nu}A^{\nu}(x))^{(+)}|\Phi\rangle = 0\,, \tag{A3}$$

where $(\partial_{\nu}A^{\nu}(x))^{(+)}$ is the positive-frequency part of $\partial_{\nu}A^{\nu}(x)$. The Heisenberg's operators $\psi(x)$, $\overline{\psi}(x)$, and $A^{\nu}(x)$ obey the same equal-time permutation relations as the corresponding free-field operators. However, in contrast to the free fields, the permutation relations for arbitrary times remain unknown. Due to the time-translation invariance, Heisenberg's operators obey the following transformation equation

$$\exp(iHt)F(0,\mathbf{x})\exp(-iHt) = F(t,\mathbf{x})\,, \tag{A4}$$

where H is the Hamiltonian of the system in the Heisenberg representation. For more details, see [20,52,74].

APPENDIX B

Let us investigate singularities of the Green function $\mathcal{G}(E)$ in a finite order of the perturbation theory. In m-th order in e, which corresponds to the order $m/2$ in α, it is given by

$$\begin{aligned}
&\mathcal{G}^{(m/2)}(E;\mathbf{x}'_1,\dots\mathbf{x}'_N;\mathbf{x}_1,\dots\mathbf{x}_N)\delta(E-E')\\
&= \frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty}dtdt'\exp(iE't'-iEt)\frac{(-i)^m}{m!}e^m\int d^4y_1\cdots d^4y_m\\
&\quad\times\langle 0|T\psi_{\rm in}(t',\mathbf{x}'_1)\cdots\psi_{\rm in}(t',\mathbf{x}'_N)\overline{\psi}_{\rm in}(t,\mathbf{x}_N)\cdots\overline{\psi}_{\rm in}(t,\mathbf{x}_1)\\
&\quad\times\overline{\psi}_{\rm in}(y_1)\gamma_{\rho}\psi_{\rm in}(y_1)A^{\rho}_{\rm in}(y_1)\cdots\overline{\psi}_{\rm in}(y_m)\gamma_{\sigma}\psi_{\rm in}(y_m)A^{\sigma}_{\rm in}(y_m)|0\rangle_{\rm con}\,,
\end{aligned} \tag{B1}$$

where the label "con" means that disconnected vacuum-vacuum subdiagrams must be omitted. For simplicity, we omit here the mass renormalization counterterm. The presence of this term would not change the consideration given below.

Let us consider the contribution of a diagram of m-th order in e. This diagram is defined by a certain order of contractions in equation (B1). The contractions between the electron-positron fields and between the photon fields give the propagators (2.10) and (2.11), respectively. In this Appendix we will use the following representation for these propagators

$$\begin{aligned}
\langle 0|T\psi_{\rm in}(x)\overline{\psi}_{\rm in}(y)|0\rangle &= \theta(x^0-y^0)\sum_{\varepsilon_n>0}\psi_n(\mathbf{x})\overline{\psi}_n(\mathbf{y})\exp[-i\varepsilon_n(x^0-y^0)]\\
&\quad-\theta(y^0-x^0)\sum_{\varepsilon_n<0}\psi_n(\mathbf{x})\overline{\psi}_n(\mathbf{y})\exp[-i\varepsilon_n(x^0-y^0)]\,,
\end{aligned} \tag{B2}$$

$$\langle 0|TA^{\rho}_{\rm in}(x)A^{\sigma}_{\rm in}(y)|0\rangle = -g^{\rho\sigma}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{\exp[-i\sqrt{\mathbf{k}^2+\mu^2}|x^0-y^0|]\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]}{2\sqrt{\mathbf{k}^2+\mu^2}}\,. \tag{B3}$$

Here, by definition, $\theta(t) = (t+|t|)/(2t)$ for $t\neq 0$ and $\theta(0) = 1/2$, and a non-zero photon mass is introduced. Following to [81,12], to investigate the singularities of $\mathcal{G}^{(m/2)}(E)$ we will use the formalism of time-ordered diagrams [82,83]. Let us consider a certain order of the time variables

$$y^0_{i_m} > y^0_{i_{m-1}} > \cdots y^0_{i_l} > t' > y^0_{i_{l-1}} > \cdots y^0_{i_s} > t > y^0_{i_{s-1}} > \cdots y^0_{i_1}$$

which defines a time-ordered version of the Feynman diagram. The contribution of the Feynman diagram is the sum of all time-ordered versions. Every time-ordered version is conveniently represented by a diagram in which the verteces are ordered upwards according to the time increase (see, for example, Fig. 35). According to equations (B2) and (B3), every electron propagator contains a sum over the whole electron-energy spectrum and every photon propagator contains an integral over the photon momentum. Let us put these sums and integrals in front of the expression for the time-ordered version of the Feynman diagram under consideration. Then, an electron line is characterized by an electron energy ε_n and, according to (B2), gives a factor (here we are interested only in time-dependent terms)

$$\exp\left[-i\varepsilon_n(y_i^0-y_k^0)\right]=\exp\left[-i|\varepsilon_n|(y_i^0-y_k^0)\right]\quad\text{for}\quad\varepsilon_n>0$$

and

$$-\exp\left[i\varepsilon_n(y_i^0-y_k^0)\right]=-\exp\left[-i|\varepsilon_n|(y_i^0-y_k^0)\right]\quad\text{for}\quad\varepsilon_n<0\,,$$

where in both case we consider $y_i^0>y_k^0$. A photon line gives a factor

$$\exp\left[-i\sqrt{\mathbf{k}^2+\mu^2}\,(y_i^0-y_k^0)\right],$$

where we consider again $y_i^0>y_k^0$. Every time y_i^0 on the diagram is marked by a horizontal dashed line. These lines may intersect other electron and photon lines (see Fig. 35). For the point of intersection with an electron line we introduce a factor $\exp(i|\varepsilon_n|y_i^0)\exp(-i|\varepsilon_n|y_i^0)=1$, where ε_n is the energy of the intersected electron. For the point of intersection with a photon line we introduce a factor $\exp(i\sqrt{\mathbf{k}^2+\mu^2}\,y_i^0)\exp(-i\sqrt{\mathbf{k}^2+\mu^2}\,y_i^0)=1$, where $\mathbf{k}$ is the momentum of the intersected photon. In addition, we represent the factor $\exp(iE't')\exp(-iEt)$ as

$$\begin{aligned}\exp(iE't')\exp(-iEt)=&\exp\left[i(E'-E)y_{i_m}^0\right]\exp\left[-i(E'-E)y_{i_m}^0\right]\cdots\\&\times\exp\left[i(E'-E)y_{i_l}^0\right]\exp\left[-i(E'-E)y_{i_l}^0\right]\\&\times\exp(iE't')\exp(-iEt')\exp(iEt')\exp(-iEy_{i_{l-1}}^0)\\&\times\exp(iEy_{i_{l-1}}^0)\exp(-iEy_{i_{l-2}}^0)\cdots\exp(iEy_{i_s}^0)\exp(-iEt)\,.\end{aligned}\tag{B4}$$

As a result of all the representations the integral over times at fixed intermediate electron states (n) and the photon momenta ($\mathbf{k}$) is

$$\begin{aligned}I_m\equiv&\int_{-\infty}^{\infty}dy_{i_m}^0\int_{-\infty}^{y_{i_m}^0}dy_{i_{m-1}}^0\cdots\int_{-\infty}^{y_{i_l}^0}dt'\int_{-\infty}^{t'}dy_{i_{l-1}}^0\cdots\int_{-\infty}^{y_{i_s}^0}dt\int_{-\infty}^{t}dy_{i_{s-1}}^0\cdots\int_{-\infty}^{y_{i_2}^0}dy_{i_1}^0\\&\times\exp\left[i(E'-E)y_{i_m}^0\right]\exp\left[i(E-E'-\sum_{(m)}|\varepsilon_n|-\sum_{(m)}\sqrt{\mathbf{k}^2+\mu^2})(y_{i_m}^0-y_{i_{m-1}}^0)\right]\cdots\\&\times\exp\left[i(E-E'-\sum_{(l)}|\varepsilon_n|-\sum_{(l)}\sqrt{\mathbf{k}^2+\mu^2})(y_{i_l}^0-t')\right]\\&\times\exp\left[i(E-\sum_{(t')}|\varepsilon_n|-\sum_{(t')}\sqrt{\mathbf{k}^2+\mu^2})(t'-y_{i_{l-1}}^0)\right]\cdots\\&\times\exp\left[i(E-\sum_{(s)}|\varepsilon_n|-\sum_{(s)}\sqrt{\mathbf{k}^2+\mu^2})(y_{i_s}^0-t)\right]\\&\times\exp\left[i(-\sum_{(t)}|\varepsilon_n|-\sum_{(t)}\sqrt{\mathbf{k}^2+\mu^2})(t-y_{i_{s-1}}^0)\right]\cdots\\&\times\exp\left[i(-\sum_{(2)}|\varepsilon_n|-\sum_{(2)}\sqrt{\mathbf{k}^2+\mu^2})(y_{i_2}^0-y_{i_1}^0)\right].\end{aligned}\tag{B5}$$

Here $\sum_{(m)}|\varepsilon_n|$ denotes the sum of the electron energies from the electron lines which are sandwiched between the horizontal lines corresponding to the times $y_{i_m}^0$ and $y_{i_{m-1}}^0$. $\sum_{(m)}\sqrt{\mathbf{k}^2+\mu^2}$ denotes the sum of the photon energies from the photon lines which are sandwiched between the horizontal lines corresponding to the times $y_{i_m}^0$ and $y_{i_{m-1}}^0$. Using the identity

$$\int_{-\infty}^{0}dx\exp(-i\alpha x)=\frac{i}{\alpha+i0}\tag{B6}$$

one easily finds

$$I_m = 2\pi\delta(E-E')\frac{i}{-\sum_{(m)}|\varepsilon_n| - \sum_{(m)}\sqrt{\mathbf{k}^2+\mu^2}}\cdots\frac{i}{-\sum_{(l)}|\varepsilon_n| - \sum_{(l)}\sqrt{\mathbf{k}^2+\mu^2}}$$
$$\times\frac{i}{E-\sum_{(t')}|\varepsilon_n| - \sum_{(t')}\sqrt{\mathbf{k}^2+\mu^2}+i0}\cdots\frac{i}{E-\sum_{(s)}|\varepsilon_n| - \sum_{(s)}\sqrt{\mathbf{k}^2+\mu^2}+i0}$$
$$\times\frac{i}{-\sum_{(t)}|\varepsilon_n| - \sum_{(t)}\sqrt{\mathbf{k}^2+\mu^2}}\cdots\frac{i}{-\sum_{(2)}|\varepsilon_n| - \sum_{(2)}\sqrt{\mathbf{k}^2+\mu^2}}\,. \tag{B7}$$

A similar calculation for $t' < t$ yields an expression which is obtained from (B7) by a replacement $E \to -E$ in all the denominators.

Taking into account that every photon line contracts two vertices, one obtains that at least $m/2$ denominators in (B7) have to contain the photon-energy terms and, therefore, do not contribute to the singularities under consideration. It follows that $\mathcal{G}^{(m/2)}(E)$ has isolated poles of all orders till $m/2+1$ at the unperturbed positions of the bound state energies. The separation of the poles from the related cuts is provided by keeping non-zero photon mass μ. As to the cuts starting from the lower energy levels, they can be turned down.

APPENDIX C

To prove the equation (2.56) we have to show that

$$\mathcal{G}(E)\delta(E-E') = \frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0$$
$$\times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0)$$
$$\times G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0)\,, \tag{C1}$$

where, for short, the space variables are omitted. According to the definition of G (see equation (2.12)) equation (C1) is equivalent to the following

$$\mathcal{G}(E)\delta(E-E') = \frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0$$
$$\times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0)$$
$$\times(2\pi)^{-2N}\int_{-\infty}^{\infty} dx_1^0\cdots dx_N^0 dx_1'^0\cdots dx_N'^0$$
$$\times\exp\left(ip_1'^0x_1'^0+\cdots+ip_N'^0x_N'^0-ip_1^0x_1^0-\cdots-ip_N^0x_N^0\right)$$
$$\times\langle 0|T\psi(x_1')\cdots\psi(x_N')\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle$$
$$= (2\pi)^{-2N}\frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_2^0\cdots dp_N^0 dp_2'^0\cdots dp_N'^0$$
$$\times\int_{-\infty}^{\infty} dx_1^0\cdots dx_N^0 dx_1'^0\cdots dx_N'^0$$
$$\times\exp\left[i(E'-p_2'^0-\cdots-p_N'^0)x_1'^0+ip_2'^0x_2'^0\cdots+ip_N'^0x_N'^0\right]$$
$$\times\exp\left[-i(E-p_2^0-\cdots-p_N^0)x_1^0-ip_2^0x_2^0-\cdots-ip_N^0x_N^0\right]$$
$$\times\langle 0|T\psi(x_1')\cdots\psi(x_N')\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle\,. \tag{C2}$$

Using the identity

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\exp\left(i\omega x\right) = \delta(x) \tag{C3}$$

we obtain

$$\mathcal{G}(E)\delta(E-E') = (2\pi)^{-2}\frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dx_1^0\cdots dx_N^0 dx_1'^0\cdots dx_N'^0\delta(x_1'^0-x_2'^0)\cdots\delta(x_1'^0-x_N'^0)$$
$$\times\delta(x_1^0-x_2^0)\cdots\delta(x_1^0-x_N^0)\exp\left(iE'x_1'^0-iEx_1^0\right)$$
$$\times\langle 0|T\psi(x_1')\cdots\psi(x_N')\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle$$
$$= \frac{1}{2\pi i}\frac{1}{N!}\int_{-\infty}^{\infty} dx^0 dx'^0\exp\left(iE'x'^0-iEx^0\right)$$
$$\times\langle 0|T\psi(x'^0,\mathbf{x}_1')\cdots\psi(x'^0,\mathbf{x}_N')\overline{\psi}(x^0,\mathbf{x}_N)\cdots\overline{\psi}(x^0,\mathbf{x}_1)|0\rangle\,. \tag{C4}$$

The last equation exactly coincides with the definition of $\mathcal{G}(E)$ given by (2.18).

APPENDIX D

To derive the equation (2.61) we use the following two identities. First, if A is a symmetric operator in coordinates of all the electrons, one obtains (see, e.g., [84])

$$A_{ik}\equiv\langle u_i|A|u_k\rangle = \sum_P(-1)^P\psi^*_{Pi_1}(\xi_1')\cdots\psi^*_{Pi_N}(\xi_N')A(\xi_1',\ldots,\xi_N';\xi_1,\ldots,\xi_N)$$
$$\times\psi_{k_1}(\xi_1)\cdots\psi_{k_N}(\xi_N)\,, \tag{D1}$$

where repeated variables $\{\xi\}$ imply integration (the integration over $\mathbf{x}$ and the summation over α), $A(\xi_1',\ldots,\xi_N';\xi_1,\ldots,\xi_N)$ is the kernel of the operator A. Second, if the kernel of the operator A is represented in the form

$$A(\xi_1',\ldots,\xi_N';\xi_1,\ldots,\xi_N) = \sum_Q(-1)^Q a(\xi_{Q1}',\ldots,\xi_{QN}';\xi_1,\ldots,\xi_N)\,, \tag{D2}$$

one can find

$$A_{ik} = N!\sum_P(-1)^P\psi^*_{Pi_1}(\xi_1')\cdots\psi^*_{Pi_N}(\xi_N')a(\xi_1',\ldots,\xi_N';\xi_1,\ldots,\xi_N)$$
$$\times\psi_{k_1}(\xi_1)\cdots\psi_{k_N}(\xi_N)\,. \tag{D3}$$

According to (2.60) we have

$$\mathcal{G}(E)\gamma_1^0\cdots\gamma_N^0\delta(E-E') = \frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0$$
$$\times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0)$$
$$\times\sum_P(-1)^P\widehat{G}((p_{P1}'^0,\xi_{P1}'),\ldots,(p_{PN}'^0,\xi_{PN}');(p_1^0,\xi_1),\ldots,(p_N^0,\xi_N))$$
$$= \frac{2\pi}{i}\frac{1}{N!}\sum_P(-1)^P\int_{-\infty}^{\infty} dp_1'^0\cdots dp_N'^0 dp_1^0\cdots dp_N^0$$
$$\times\delta(E-p_1^0-\cdots-p_N^0)\delta(E'-p_1'^0-\cdots-p_N'^0)$$
$$\times\widehat{G}((p_1'^0,\xi_{P1}'),\ldots,(p_N'^0,\xi_{PN}');(p_1^0,\xi_1),\ldots,(p_N^0,\xi_N))$$
$$\equiv\sum_P(-1)^P\tilde{G}(\xi_{P1}',\ldots,\xi_{PN}';\xi_1,\ldots,\xi_N)\,. \tag{D4}$$

Using (D1)-(D4) one easily obtains (2.61).

APPENDIX E

Let us consider the function $G(E',E)$ defined as

$$G(E',E) = \int_{-\infty}^{\infty} dtdt'\exp\left(iE't'-iEt\right)\langle 0|TA(t')B(0)C(t)|0\rangle\,. \tag{E1}$$

Using the transformation rules for the Heisenberg operators and integrating over the time variables one can derive the following double spectral representation for $G(E', E)$

$$
\begin{aligned}
G(E', E) = &- \int_{-\infty}^{\infty} dW' dW \Big[\frac{K(W', W)}{(E' - W')(E - W)} + \frac{L(W', W)}{(E' + W')(E + W)} \Big] \\
&+ \int_{-\infty}^{\infty} dW' d\omega \Big[\frac{M(W', \omega)}{(E' - W')(k^0 + \omega)} + \frac{N(W', \omega)}{(E' + W')(k^0 - \omega)} \Big] \\
&- \int_{-\infty}^{\infty} d\omega dW \Big[\frac{P(\omega, W)}{(k^0 - \omega)(E - W)} + \frac{Q(\omega, W)}{(k^0 + \omega)(E + W)} \Big] ,
\end{aligned}
\tag{E2}
$$

where $k^0 = E - E'$,

$$K(W', W) = \sum_{n,m} \delta(W' - E_n) \delta(W - E_m) \langle 0|A(0)|n\rangle \langle n|B(0)|m\rangle \langle m|C(0)|0\rangle \,, \tag{E3}$$

$$L(W', W) = \sum_{n,m} \delta(W' - E_n) \delta(W - E_m) \langle 0|C(0)|n\rangle \langle n|B(0)|m\rangle \langle m|A(0)|0\rangle \,, \tag{E4}$$

$$M(W', \omega) = \sum_{n,m} \delta(W' - E_n) \delta(\omega - E_m) \langle 0|A(0)|n\rangle \langle n|C(0)|m\rangle \langle m|B(0)|0\rangle \,, \tag{E5}$$

$$N(W', \omega) = \sum_{n,m} \delta(W' - E_m) \delta(\omega - E_n) \langle 0|B(0)|n\rangle \langle n|C(0)|m\rangle \langle m|A(0)|0\rangle \,, \tag{E6}$$

$$P(\omega, W) = \sum_{n,m} \delta(\omega - E_n) \delta(W - E_m) \langle 0|B(0)|n\rangle \langle n|A(0)|m\rangle \langle m|C(0)|0\rangle \,, \tag{E7}$$

$$Q(\omega, W) = \sum_{n,m} \delta(\omega - E_m) \delta(W - E_n) \langle 0|C(0)|n\rangle \langle n|A(0)|m\rangle \langle m|B(0)|0\rangle \,. \tag{E8}$$

---

[1] H.F. Beyer, V.P. Shevelko (Eds.), Atomic Physics with Heavy Ions, Springer, Berlin, 1999.
[2] V.M. Shabaev, A.N. Artemyev, V.A. Yerokhin, Phys. Scr. T 86 (2000) 7.
[3] P.J. Mohr, G. Plunien, G. Soff, Phys. Rep. 293 (1998) 227.
[4] J. Sapirstein, in: D.H.E. Dubin, D. Schneider (Eds.), Trapped Charged Particles and Fundamental Physics, American Institute of Physics Conference Proceedings 457, 1999, p. 3.
[5] T. Beier, Phys. Rep., in press.
[6] I. Lindgren, Phys. Scr. T 80 (1999) 131.
[7] M. Gell-Mann, F. Low, 1951 Phys. Rev. 84 (1951) 350.
[8] J. Sucher, Phys. Rev. 107 (1957) 1448.
[9] L.N. Labzowsky, Zh. Eksp. Teor. Fiz. 59 (1970) 168 [Sov. Phys. JETP 32 (1970) 94].
[10] M.A. Braun, A.D. Gurchumelia, Teor. Mat. Fiz. 45 (1980) 199 [Theor. Math. Phys. 45 (1980) N 2].
[11] Yu.Yu. Dmitriev, G.L. Klimchitskaya, L.N. Labzowsky, Relativistic Effects in Spectra of Atomic Systems, Energoatomizdat, Moscow, 1984.
[12] M.A. Braun, A.D. Gurchumelia, U.I. Safronova, Relativistic Atom Theory, Nauka, Moscow, 1984.
[13] P.J. Mohr, in: W.R. Johnson, P.J. Mohr, J. Sucher (Eds.), Relativistic, Quantum Electrodynamics and Weak Interaction Effects in Atoms, American Institute of Physics Conference Series no 189, 1989, p. 47.
[14] I. Lindgren, in: W.R. Johnson, P.J. Mohr, J. Sucher (Eds.), Relativistic, Quantum Electrodynamics and Weak Interaction Effects in Atoms, American Institute of Physics Conference Series no 189, 1989, p. 371.
[15] L. Labzowsky, G. Klimchitskaya, Yu. Dmitriev, Relativistic Effects in Spectra of Atomic Systems, IOP Publishing, Bristol, 1993.
[16] J. Sapirstein, Rev. Mod. Phys. 70 (1998) 55.
[17] F.J. Dyson, Phys. Rev. 75 (1949) 486, 1736.
[18] E.E. Salpeter, H.A. Bethe, 1951 Phys. Rev. 84 (1951) 1232.
[19] J. Hubbard, Proc. Roy. Soc. A 240 (1957) 539.

[20] S.S. Schweber, An Introduction to Relativistic Quantum Field Theory, Harper & Row, New York, 1961.
[21] A.N. Vasil'ev, A.L. Kitanin, Teor. Mat. Fiz. 24 (1975) 219 [Theor. Math. Phys. 24 (1975) N 2].
[22] S.A. Zapryagaev, N.L. Manakov, V.G. Pal'chikov, Theory of One- and Two-Electron Multicharged Ions Energoatomizdat, Moscow, 1985.
[23] J. Sapirstein, Phys. Scr. 36 (1987) 801.
[24] C. Itzykson, J.-B. Zuber, Quantum Field Theory, McGraw-Hill, New York, 1980.
[25] V.M. Shabaev, in : U.I. Safronova (Ed.), Many-particles Effects in Atoms, AN SSSR, Nauchnyi Sovet po Spektroskopii, Moscow, 1988, p. 15.
[26] V.M. Shabaev, in : U.I. Safronova (Ed.), Many-particles Effects in Atoms, AN SSSR, Nauchnyi Sovet po Spektroskopii, Moscow, 1988, p. 24.
[27] V.M. Shabaev, Izv. Vuz. Fiz. 33 (1990) 43 [Sov. Phys. Journ. 33 (1990) 660].
[28] V.M. Shabaev, Teor. Mat. Fiz. 82 (1990) 83 [Theor. Math. Phys. 82 (1990) 57].
[29] V.M. Shabaev, J. Phys. A 24 (1991) 5665.
[30] V.V. Karasiov, L.N. Labzowsky, A.V. Nefiodov, V.M. Shabaev, Phys. Lett. A 161 (1992) 453.
[31] V.M. Shabaev, J. Phys. B 26 (1993) 4703.
[32] V.M. Shabaev, I.G. Fokeeva, Phys. Rev. A 49 (1994) 4489.
[33] V.M. Shabaev, Phys. Rev. A 50 (1994) 4521.
[34] M.B. Shabaeva, V.M. Shabaev, Phys. Rev. A 52 (1995) 2811.
[35] V.A. Yerokhin, A.N. Artemyev, V.M. Shabaev, Phys. Lett. A 234 (1997) 361.
[36] A.N. Artemyev, V.M. Shabaev, V.A. Yerokhin, Phys. Rev. A 56 (1997) 3529.
[37] V.M. Shabaev, Phys. Rev. A 57 (1998) 59.
[38] A.N. Artemyev, T. Beier, G. Plunien, V.M. Shabaev, G. Soff, V.A. Yerokhin, Phys. Rev. A 60 (1999) 45.
[39] V.A. Yerokhin, A.N. Artemyev, T. Beier, G. Plunien, V.M. Shabaev, G. Soff, Phys. Rev. A 60 (1999) 3522.
[40] A.N. Artemyev, T. Beier, G. Plunien, V.M. Shabaev, G. Soff, V.A. Yerokhin, Phys. Rev. A, in press.
[41] V.M. Shabaev, V.A. Yerokhin, T. Beier, J. Eichler, Phys. Rev. A 61 (2000) 052112.
[42] V.A. Yerokhin, V.M. Shabaev, T. Beier, J. Eichler, Phys. Rev. A, in press.
[43] M.A. Braun, A.S. Shirokov, Izv. Akad. Nauk SSSR: Ser. Fiz. 41 (1977) 2585 [Bull. Acad. Sci. USSR: Phys. Ser. 41 (1977) 109].
[44] M.A. Braun, Kh. Parera, Izv. Akad. Nauk SSSR: Ser. Fiz. 50 (1986) 1303 [Bull. Acad. Sci. USSR: Phys. Ser. 50 (1986) 59]
[45] M.A. Braun, Teor. Mat. Fiz. 72 (1987) 394 [Theor. Math. Phys. 72 (1987) 958].
[46] V.M. Shabaev, Teor. Mat. Fiz. 63 (1985) 394 [Theor. Math. Phys. 63 (1985) 588].
[47] V.M. Shabaev, Yad. Fiz. 47 (1988) 107 [Sov. J. Nucl. Phys. 47 (1988) 69].
[48] S.A. Zapryagaev, D.I. Morgulis Yad. Fiz. 45 (1987) 716 [Sov. J. Nucl. Phys. 45 (1987) N 3].
[49] G. Feldman, T. Fulton, Ann. Phys. (N.Y.) 179 (1987) 20.
[50] T. Fulton, in: W.R. Johnson, P.J. Mohr, J. Sucher (Eds.), Relativistic, Quantum Electrodynamics and Weak Interaction Effects in Atoms, American Institute of Physics Conference Series no 189, 1989, p. 429.
[51] D.R. Yennie, in: W.R. Johnson, P.J. Mohr, J. Sucher (Eds.), Relativistic, Quantum Electrodynamics and Weak Interaction Effects in Atoms, American Institute of Physics Conference Series no 189, 1989, p. 393.
[52] J.D. Bjorken, D. Drell, Relativistic Quantum Fields, McGraw-Hill, New York, 1965.
[53] P.J. Mohr, Phys. Rev. A 32 (1985) 1949.
[54] V.L. Bonch-Bruevich, S.V. Tyablikov The Green function method in Statistical Mechanics, North-Holland Publishing Company, Amsterdam, 1962.
[55] D.J. Thouless, The Quantum Mechanics of Many-Body Systems, Academic Press, New York, 1961.
[56] A.B. Migdal, Theory of finite fermi-systems and properties of atomic nuclei, Nauka, Moscow, 1983.
[57] A.A. Logunov, A.N. Tavkhelidze, Nuovo Cim. 29 (1963) 380.
[58] R.N. Faustov, Teor. Mat. Fiz. 3 (1970) 240 [Theor. Math. Phys. 3 (1970) N 2].
[59] B. Sz-Nagy, Comm. Math. Helv. 19 (1946/47) 347.
[60] T. Kato, Progr. Theor. Phys. 4 (1949) 514.
[61] T. Kato, Perturbation Theory for Linear Operators, Springer, Berlin, 1966.
[62] A. Messiah, Quantum Mechanics, Vol. 2, Wiley, New York, 1962.
[63] M. Reed, B. Simon, Methods of Modern Mathematical Physics, Vol. 4: Analysis of Operators, Academic Press, New York, 1978.
[64] G.P. Lepage, Phys. Rev. A 16 (1977) 863.
[65] S.A. Blundell, P.J. Mohr, W.R. Johnson, J. Sapirstein, Phys. Rev. A 48 (1993) 2615.
[66] I.S. Gradshtein, I.N. Ryzhyk, Tables of Integrals, Sums, Series, and Products, Nauka, Moscow, 1977.
[67] M.H. Mittleman, Phys. Rev. A 5 (1972) 2395.
[68] E.-O. Le Bigot, P. Indelicato, V.M. Shabaev, to be published.
[69] A.S. Yelkhovsky, Budker Institute of Nuclear Physics, Report No. BINP 94-27, Novosibirsk, 1994; e-print hep-th/9403095; Zh. Eksp. Teor. Fiz. 110 (1996) 431 [JETP 83 (1996) 230].
[70] K. Pachucki, H. Grotch, Phys. Rev. A 51 (1995) 1854.

[71] N.N. Bogolyubov, D.V. Shirkov, Introduction to the Theory of Quantized Fields, Nauka, Moscow, 1984.
[72] V.B. Berestetsky, E.M. Lifshitz, L.P. Pitaevsky, Quantum Electrodynamics, Pergamon Press, Oxford, 1982.
[73] P. Indelicato, V.M. Shabaev, to be published.
[74] A.I. Akhiezer, V.B. Berestetskii, Quantum Electrodynamics, Nauka, Moscow, 1969.
[75] F.E. Low, Phys. Rev. 88 (1952) 53.
[76] M. A. Braun, Zh. Eksp. Teor. Fiz. 94 (1988) 145.
[77] V.G. Gorshkov, L.N. Labzowsky, A.A. Sultanaev, Zh. Eksp. Teor. Fiz. 96 (1989) 53 [Sov. Phys. JETP 69 (1989) 28].
[78] A.V. Nefiodov, V.V. Karasiov, V.A. Yerokhin, Phys. Rev. A 50 (1994) 4975.
[79] V.A. Yerokhin, A.N. Artemyev, V.M. Shabaev, M.M. Sysak, O.M. Zherebtsov, G. Soff, to be published.
[80] V.M. Shabaev, unpublished.
[81] A.S. Shirokov, Candidate of Science thesis, Leningrad State University, Leningrad, 1981.
[82] L. Van Hove, Physica 21 (1955) 901.
[83] N.M. Hugenholtz, Physica 23 (1957) 481.
[84] H.A. Bethe, Intermediate Quantum Mechanics, Benjamin, New York, 1964.

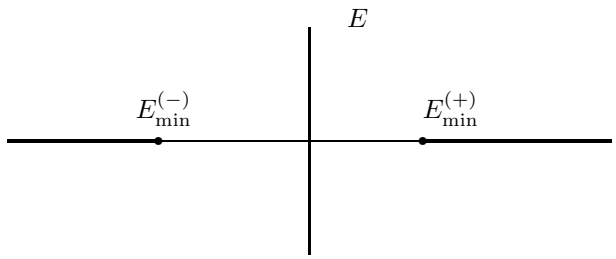


FIG. 1. Singularities of the two-time Green function in the complex E plane.

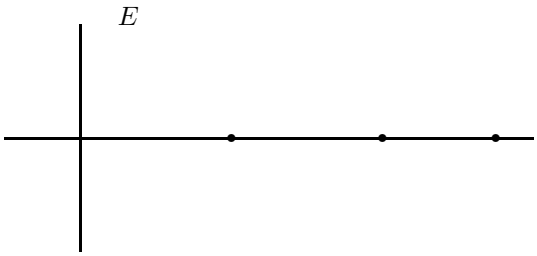


FIG. 2. Singularities of the two-time Green function in the bound state region, when the interaction between the electron-positron field and the electromagnetic field is switched off.

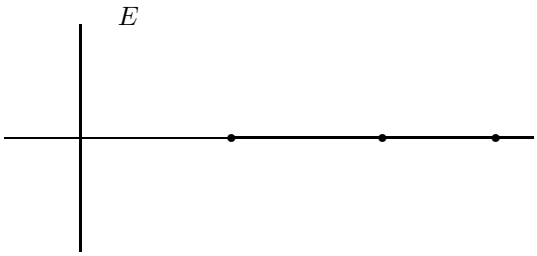


FIG. 3. Singularities of the two-time Green function in the bound state region, disregarding the instability of excited states.

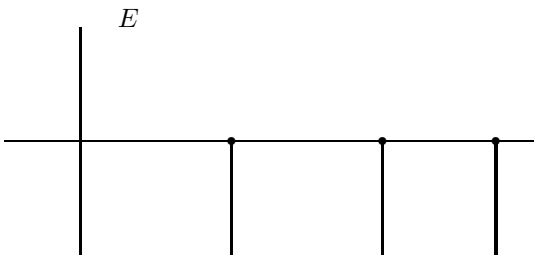


FIG. 4. Singularities of the two-time Green function in the bound state region when the cuts are turned down, to the second sheet of the Riemann surface. The instability of excited states is disregarded.

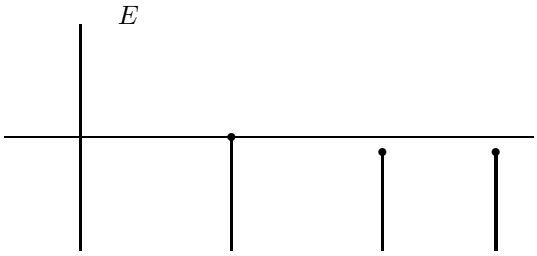


FIG. 5. Singularities of the two-time Green function in the bound state region when the cuts are turned down, to the second sheet of the Riemann surface. The instability of excited states is taken into account.

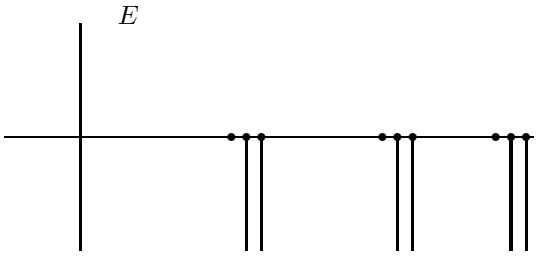


FIG. 6. Singularities of the two-time Green function in the bound state region for a non-zero photon mass, including one- and two-photon spectra, when the cuts are turned down, to the second sheet of the Riemann surface. The instability of excited states is disregarded.

FIG. 7. The contour Γ surrounds the pole corresponding to the level under consideration and keeps outside all other singularities. For simplicity, only one- and two-photon spectra are displayed.

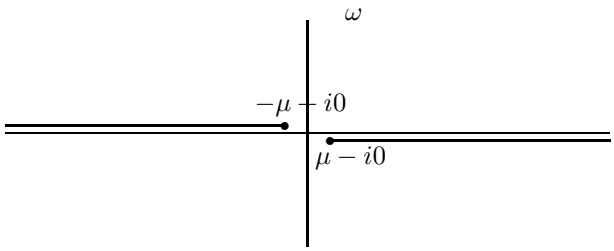


FIG. 8. Singularities of the photon propagator in the complex ω plane for a non-zero photon mass μ.

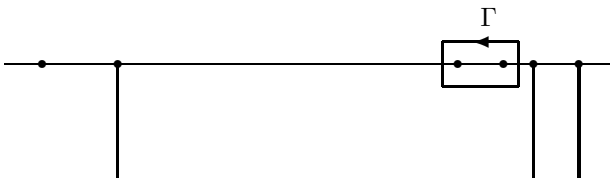


FIG. 9. The contour Γ surrounds the poles corresponding to the quasidegenerate levels under consideration and keeps outside all other singularities. For simplicity, only one-photon spectra are displayed.

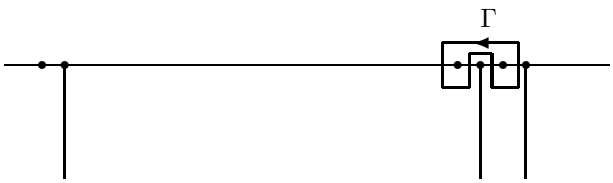


FIG. 10. A deformation of the contour Γ that allows drawing the cuts to the related poles in the case of quasidegenerate states when $\mu \to 0$. For simplicity, only one-photon spectra are displayed.

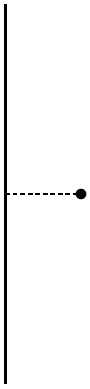


FIG. 11. The interaction with an external potential $\delta V(\mathbf{x})$.

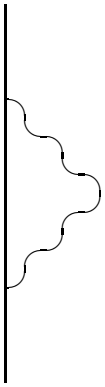


FIG. 12. The first-order self-energy diagram.

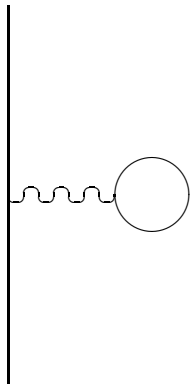


FIG. 13. The first-order vacuum-polarization diagram.

FIG. 14. The mass counterterm diagram.

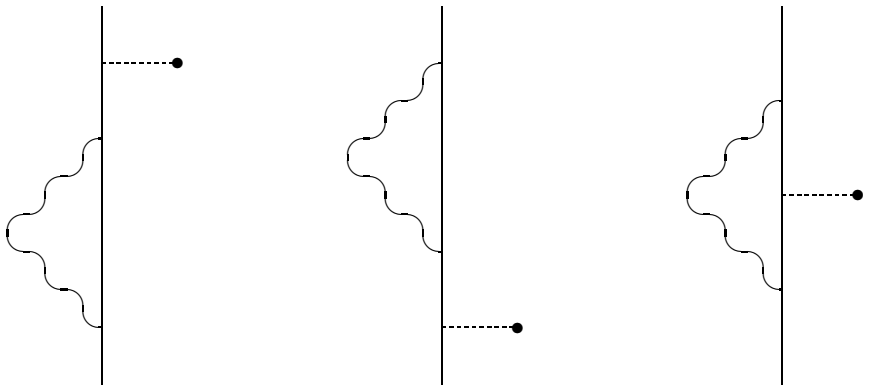


FIG. 15. δV - self energy diagrams.

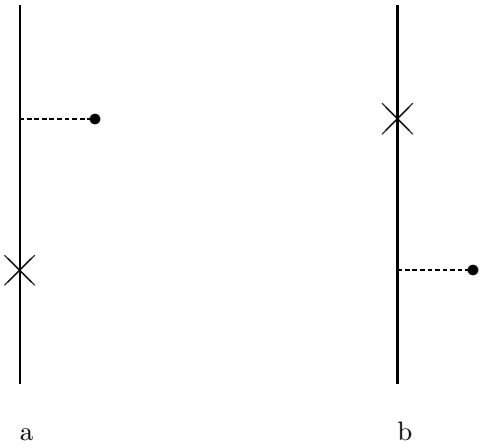


FIG. 16. δV - mass counterterm diagrams.

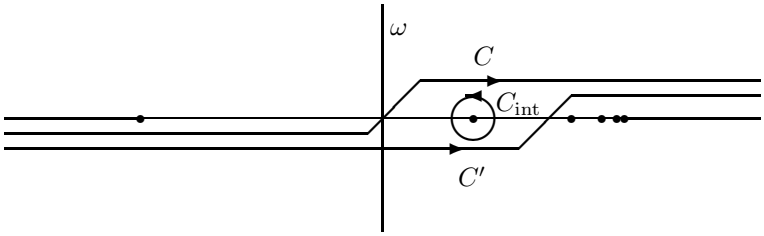


FIG. 17. C is the standard contour of the integration over the electron energy ω in the formalism with the usual vacuum. C' is the contour of the integration over ω in the formalism in which the $(1s)^2$ closed shell is referred to the vacuum. The integral along the contour $C_{\rm int} = C' - C$ describes the interaction of the valent electron with the closed shell electrons.

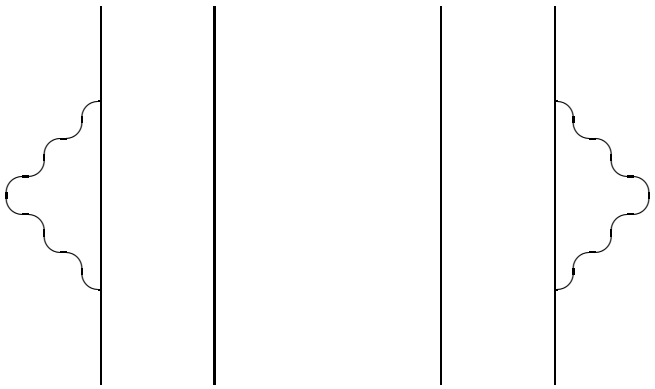


FIG. 18. The first-order self-energy diagrams for a two-electron atom.

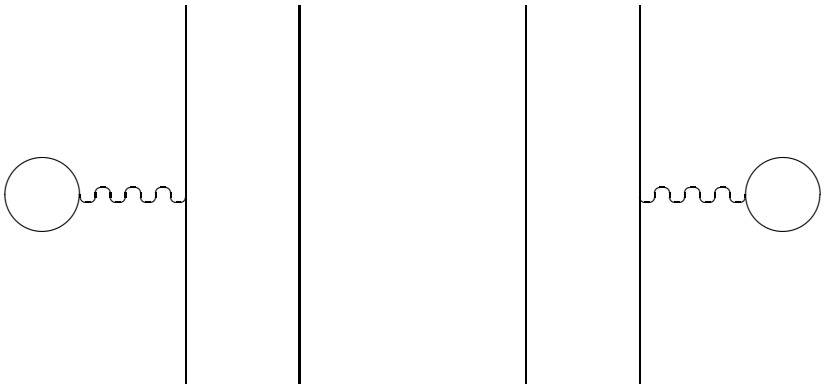


FIG. 19. The first-order vacuum-polarization diagrams for a two-electron atom.

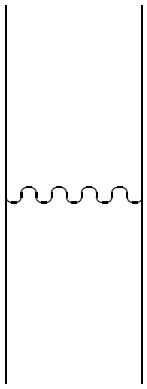


FIG. 20. One-photon exchange diagram.

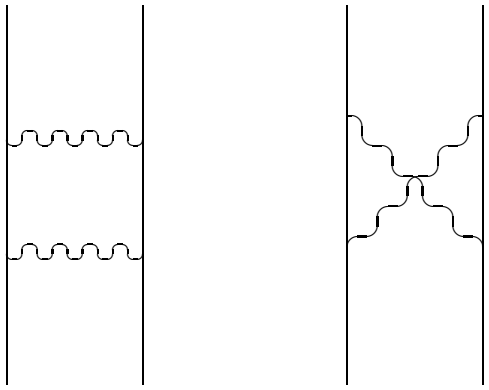


FIG. 21. Two photon exchange diagrams.

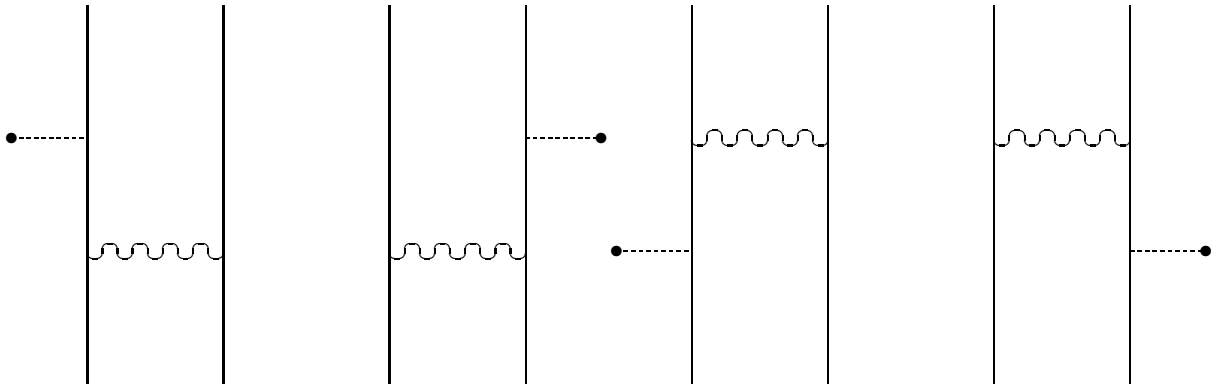


FIG. 22. δV - interelectronic-interaction diagrams.

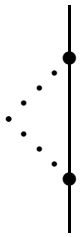


FIG. 23. Coulomb nuclear recoil diagram.

FIG. 24. One-transverse-photon nuclear recoil diagrams.

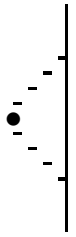


FIG. 25. Two-transverse-photon nuclear recoil diagram.

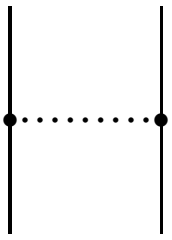


FIG. 26. Two-electron Coulomb nuclear recoil diagram.

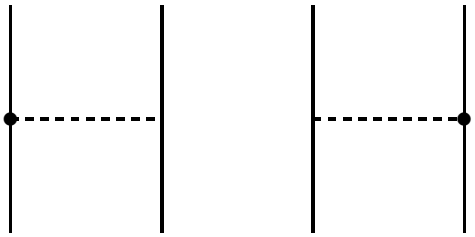


FIG. 27. Two-electron one-transverse-photon nuclear recoil diagrams.

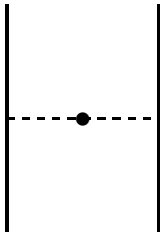


FIG. 28. Two-electron two-transverse-photon nuclear recoil diagram.

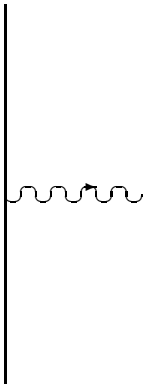


FIG. 29. The photon emission by a one-electron atom in the zeroth-order approximation.

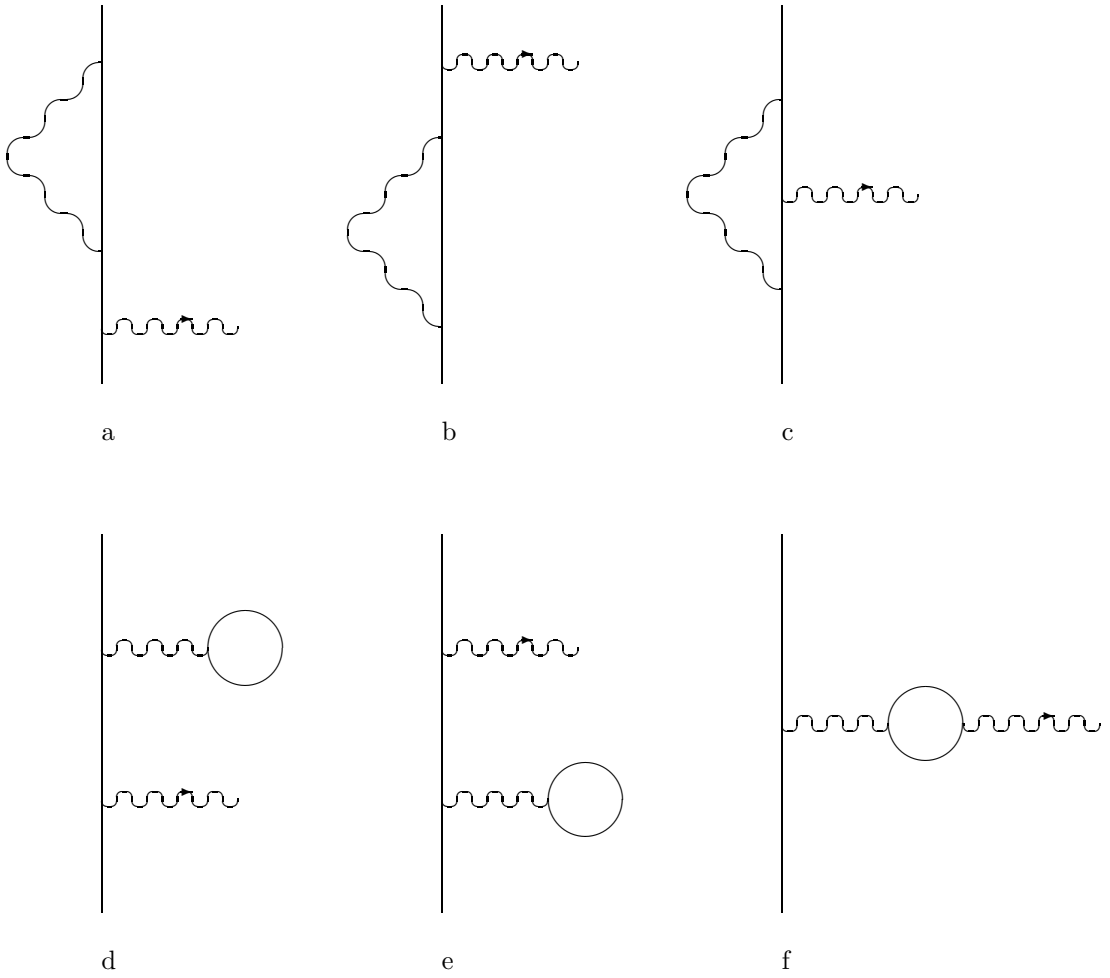


FIG. 30. The first-order QED corrections to the photon emission by a one-electron atom.

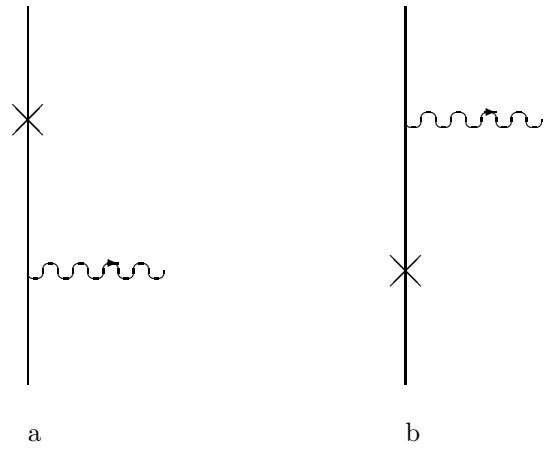


FIG. 31. The mass counterterm corrections to the photon emission by a one-electron atom.

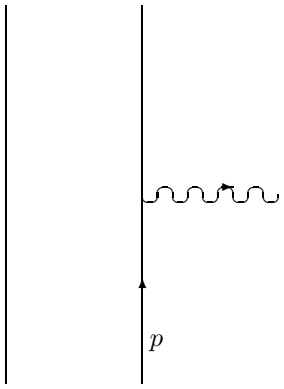


FIG. 32. The radiative recombination of an electron with a hydrogenlike atom in the zeroth-order approximation.

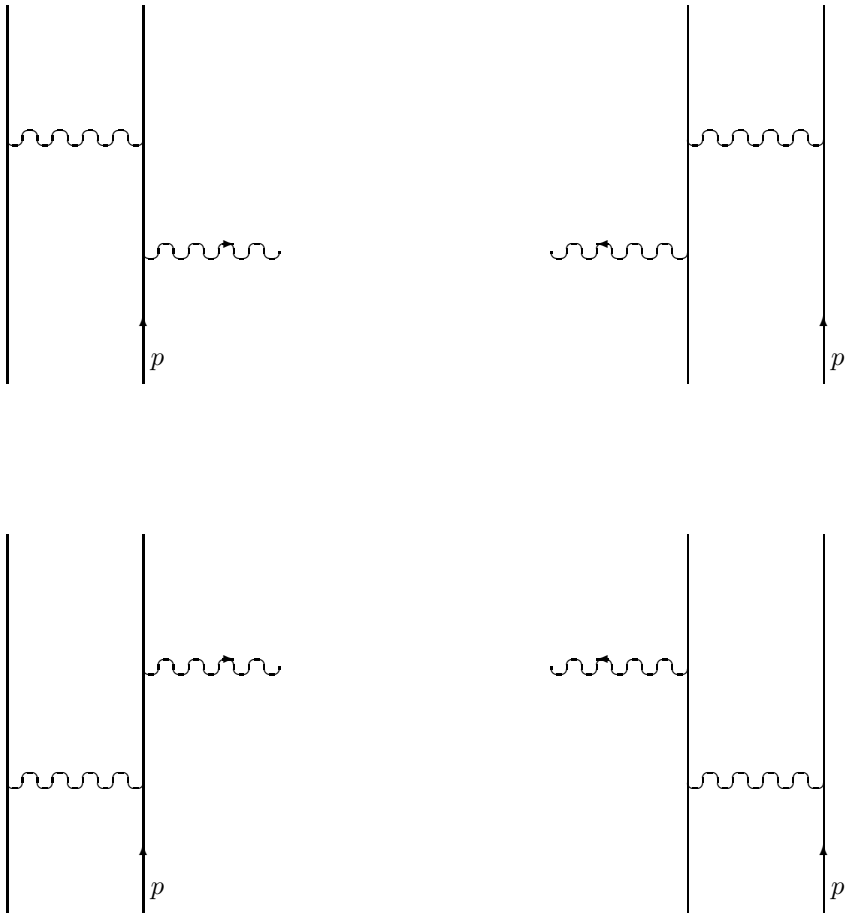


FIG. 33. The interelectronic-interaction corrections of first order in $1/Z$ to the radiative recombination of an electron with a hydrogenlike atom.

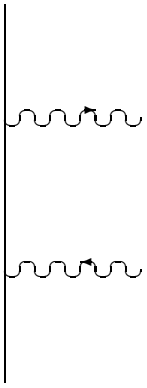


FIG. 34. The photon scattering on a one-electron atom in the zeroth-order approximation.

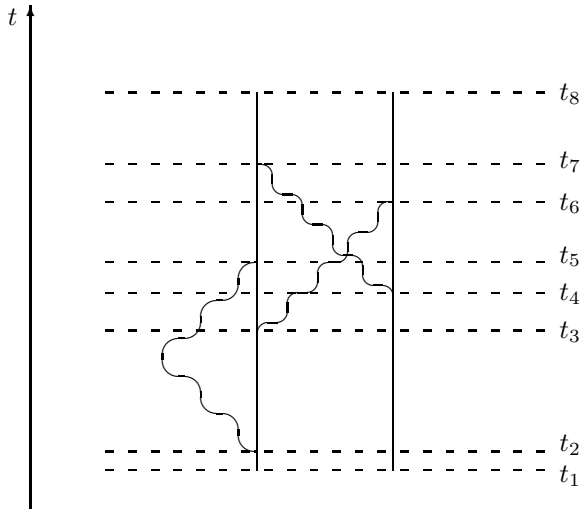


FIG. 35. A time-ordered version of a Feynman diagram.